

In the Claims:

Please cancel claims 2-7, 10, and 14-18 and amend claims 1, 8, 9, 19, and 20 as follows:

1. (Amended) A process which comprises reacting hydrogen and oxygen in a solvent in the presence of a catalyst comprising a polystyrene-polymer-encapsulated palladium transition metal to produce hydrogen peroxide, wherein the palladium is supported on a titanium zeolite prior to polystyrene encapsulation.

2-7. Cancelled.

8. (Amended) The process of claim 1 wherein the polystyrene-polymer-encapsulated palladium transition metal is produced by polymerizing styrene in an aqueous suspension in the presence of the titanium zeolite-supported palladium a transition metal source.

9. (Amended) The process of claim 1 wherein the titanium zeolite is TS-1 polymer is a phosphorus functionalized polystyrenic.

10. (Canceled).

11. (Original) The process of claim 1 wherein the solvent is selected from the group consisting of water, C₁-C₄ alcohols, carbon dioxide, and mixtures thereof.

12. (Original) The process of claim 1 wherein the solvent is a mixture of methanol and water.

13. (Original) The process of claim 12 performed in the presence of a protic acid.

14-18. (Canceled).

19. (Amended) The process of claim 13 wherein the protic acid is hydrogen bromide.

20. (Amended) The process of claim 13 wherein the protic acid is a mixture of hydrogen bromide and phosphoric acid.

=> file reg

FILE 'REGISTRY'

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FILE 'REGISTRY'

 E HYDROGEN/CN
L1 1 SEA HYDROGEN/CN
 E OXYGEN/CN
L2 1 SEA OXYGEN/CN
 E STYRENE/CN
L3 1 SEA STYRENE/CN
 E POLYSTYRENE/CN
L4 1 SEA POLYSTYRENE/CN
 E PALLADIUM/CN
L5 1 SEA PALLADIUM/CN
 E PLATINUM/CN
L6 1 SEA PLATINUM/CN
 E NICKEL/CN
L7 1 SEA NICKEL/CN
 E TITANIUM ZEOLITE/CN
L8 109 SEA ZEOLITE#
L9 5 SEA L8 AND (TITANIUM# OR TI OR TI/ELS)
 E TS-1/CN
 E TZ-1/CN

FILE 'LCA'

L10 226 SEA (ZEOLITE# OR ANALCIME# OR WAIRAKITE# OR POLLUCITE# OR
 SODALITE# OR ZK5 OR ZSM5 OR (ZK OR ZSM) (W) 5 OR LINDE# (W) A
 OR FAUJASITE# OR CHABAZITE# OR GMELINITE# OR ERIONITE#
 OR OFFRETITE# OR LEVYNITE# OR NATROLITE# OR SCOLECITE#
 OR MESOLITE#) /BI, AB
L11 18 SEA (EDINGTONITE# OR THOMSONITE# OR GONNARDITE# OR
 PHILLIPSITE# OR STILBITE# OR HARMOTOME# OR GISMONDINE#
 OR GARRONITE# OR MORDENITE# OR DACHIARDITE# OR ACHIARDITE
 # OR HEULANDITE# OR BREWSTERITE# OR EPISTILBITE# OR
 YUGAWARALITE# OR LAUMONTITE#) /BI, AB
L12 1 SEA (FERRIERITE# OR PAULINGITE#) /BI, AB

FILE 'HCA'

L13 2954 SEA L9 OR (TS OR TZ) (A) 1 OR (TITANIUM# OR TI) (2A) (ZEOLITE
 # OR L10 OR L11 OR L12)

L14 121440 SEA L5 OR (PALLADIUM# OR PD) (2A) (ENCAPSUL? OR CAPSUL? OR MICROCAPSUL? OR MICROENCAPSUL? OR SUPPORT? OR BED OR BEDS OR BEDDED OR BEDDING# OR HETEROG? OR CAT# OR CATALY?)

L15 150974 SEA L6 OR (PLATINUM# OR PT) (2A) (ENCAPSUL? OR CAPSUL? OR MICROCAPSUL? OR MICROENCAPSUL? OR SUPPORT? OR BED OR BEDS OR BEDDED OR BEDDING# OR HETEROG? OR CAT# OR CATALY?)

L16 346352 SEA L7 OR (NICKEL# OR NI) (2A) (ENCAPSUL? OR CAPSUL? OR MICROCAPSUL? OR MICROENCAPSUL? OR SUPPORT? OR BED OR BEDS OR BEDDED OR BEDDING# OR HETEROG? OR CAT# OR CATALY?)

L17 120757 SEA ENCAPSUL? OR CAPSUL? OR MICROCAPSUL? OR MICROENCAPSUL?

L18 1105 SEA (L3 OR L4 OR STYRENE# OR POLYSTYRENE# OR ?STYRYL?) (2A) (ENCAPSUL? OR CAPSUL? OR MICROCAPSUL? OR MICROENCAPSUL?)

L19 387917 SEA L3 OR L4 OR STYRENE# OR POLYSTYRENE# OR ?STYRYL?

L20 804400 SEA L1 OR H2 OR HYDROGENA? OR (HYDROGEN# OR H) (2A) (ATMOS? OR ATM# OR GAS## OR GASEOUS? OR GASIF? OR FURNISH? OR SOURC? OR SUPPLY? OR SUPPLIED OR APPLY? OR APPLIED OR APPLICATION? OR INTRODUC? OR TREAT? OR FLOW? OR STREAM? OR PROCESS? OR INJECT? OR JET# OR SYRING? OR NEEDL? OR PORT?)

L21 1420611 SEA L2 OR O2 OR OXYGENA? OR AIR OR (OXYGEN# OR O) (2A) (ATMOS? OR ATM# OR GAS## OR GASEOUS? OR GASIF? OR FURNISH? OR SOURC? OR SUPPLY? OR SUPPLIED OR APPLY? OR APPLIED OR APPLICATION? OR INTRODUC? OR TREAT? OR FLOW? OR STREAM? OR PROCESS? OR INJECT? OR JET# OR SYRING? OR NEEDL? OR PORT?)

L22 74 SEA L13 AND L20 AND L21

L23 30 SEA L22 AND (L14 OR L15 OR L16)

L24 2 SEA L22 AND L19

L25 0 SEA L22 AND L18

L26 5 SEA L22 AND L17

L27 3 SEA L23 AND L17

FILE 'REGISTRY'

E HYDROGEN PEROXIDE/CN

L28 1 SEA "HYDROGEN PEROXIDE"/CN

FILE 'HCA'

L29 185485 SEA L28 OR (HYDROGEN# OR H) (A) PEROXIDE# OR H2O2 OR HOOH

L30 29 SEA L22 AND L29

L31 12 SEA L23 AND L29

L32 212087 SEA PEROXIDE#

L33 25 SEA L22 AND L32

L34 11 SEA L23 AND L32

L35 3466 SEA L28/P

L36 12 SEA L22 AND L35

FILE 'LCA'

L37 32138 SEA (PRODUC? OR PROD# OR GENERAT? OR MANUF? OR MFR# OR
CREAT? OR FORM## OR FORMING# OR FORMAT? OR MAKE# OR
MADE# OR MAKING# OR FABRICAT? OR SYNTHESI? OR PREPAR? OR
PREP#)/BI,AB

FILE 'HCA'

L38 55218 SEA L37(3A) (PEROXIDE# OR H2O2 OR HOOH OR L28)
L39 18 SEA L22 AND L38
L40 9 SEA (L36 OR L39) AND ((L14 OR L15 OR L16 OR L17 OR L18
OR L19))

FILE 'REGISTRY'

E HYDROGEN BROMIDE/CN
L41 1 SEA "HYDROGEN BROMIDE"/CN
E PHOSPHORIC ACID/CN
L42 1 SEA "PHOSPHORIC ACID"/CN

FILE 'HCA'

L43 7487 SEA (PROTIC# OR (PROTON? OR H) (2A) (CONTAIN? OR CONTG#)
OR BRONST? OR BROENST?) (3A)ACID#
L44 52932 SEA L41 OR (HYDROGEN# OR H) (A)BROMIDE# OR HYDROBROMIC# (A)
ACID# OR HBR
L45 142350 SEA L42 OR (ORTHOPHOSPHORIC# OR PHOSPHORIC#) (2A)ACID# OR
H3PO4
L46 1 SEA L22 AND L43
L47 0 SEA L22 AND L44
L48 1 SEA L22 AND L45
L49 740 SEA TS1 OR TZ1
L50 77 SEA (L49 OR L13) AND L20 AND L21
L51 29 SEA L50 AND (L29 OR L32)
L52 14 SEA L51 AND ((L14 OR L15 OR L16 OR L17 OR L18 OR L19) OR
PD OR PT OR NI OR L43 OR L44 OR L45)

FILE 'REGISTRY'

E METHANOL/CN
L53 1 SEA METHANOL/CN
E ETHANOL/CN
L54 1 SEA ETHANOL/CN
E N-PROPANOL/CN
L55 1 SEA N-PROPANOL/CN
E ISOPROPANOL/CN
L56 1 SEA ISOPROPANOL/CN
E N-BUTANOL/CN
L57 1 SEA N-BUTANOL/CN
E SEC-BUTANOL/CN

L58 1 SEA SEC-BUTANOL/CN
E ISOBUTANOL/CN
L59 1 SEA ISOBUTANOL/CN
E TERT-BUTANOL/CN
L60 1 SEA TERT-BUTANOL/CN
E CARBON DIOXIDE/CN
L61 1 SEA "CARBON DIOXIDE"/CN

FILE 'HCA'

L62 468142 SEA L61 OR CARBON#(A)DIOXIDE# OR CO2
L63 1550321 SEA (L53 OR L54 OR L55 OR L56 OR L57 OR L58 OR L59 OR
L60) OR ALC# OR ALCOHOL## OR MECH OR ETOH OR PROH OR
IPROH OR NPROH OR BUOH OR NBUOH OR IBUOH OR SBUOH OR
TBUOH OR METHANOL# OR ETHANOL# OR PROPANOL# OR ISOPROPANO
L# OR BUTANOL# OR ISOBUTANOL#
L64 14 SEA L51 AND (L62 OR L63)
L65 12 SEA L24 OR L26 OR L27 OR L40 OR L46 OR L48
L66 16 SEA (L31 OR L34 OR L36 OR L39 OR L52 OR L64) NOT L65
L67 20 SEA (L23 OR L30 OR L33 OR L51) NOT (L65 OR L66)

=> file hca

FILE 'HCA'

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=> d l65 1-12 cbib abs hitstr hitind

L65 ANSWER 1 OF 12 HCA COPYRIGHT 2006 ACS on STN

144:23241 Use of water-treated calcined **titanium** or vanadium
zeolites as catalysts for epoxidation of olefins. Onimus,
Wilson H.; Cooker, Bernard (Lyondell Chemical Technology, L.P.,
USA). U.S. US 6972337 B1 20051206, 6 pp. (English). CODEN:
USXXAM. APPLICATION: US 2004-918605 20040812.

AB An epoxide is produced by reacting an olefin with hydrogen peroxide
in the presence of a **titanium** or vanadium **zeolite**
pretreated by heating at a temp. > 400.degree. and contacting with
water. In another embodiment, an epoxide is produced by reacting an
olefin, hydrogen and oxygen in the presence of a noble metal-contg.
titanium or vanadium **zeolite** comprising a noble
metal and a **titanium** or vanadium **zeolite**, the
titanium or vanadium **zeolite** being pretreated by
heating at a temp. > 400.degree. and contacting with water. Thus,
titanium silicalite TS 1 was obtained by

reacting tetra-Et orthosilicate (364) and tetra-Et orthotitanate (11.2 g) with a 12.5%-aq. tetrapropylammonium hydroxide (200 g of 40%-aq. tetrapropylammonium hydroxide and 440 g of deionized water). The **TS 1** crystals were dried at 55.degree. for 2 h, and calcined in **air** by heating from 20 to 110.degree. at 10 .degree./min, holding at 110.degree. for 2 h, then heating to 550.degree. at 2 .degree./min, and holding at 550.degree. for 4 h. The calcined **TS 1** was suspended in deionized water (10% slurry) under nitrogen, followed by rapid heating to 65.degree., maintaining at 65.degree. for 7 days, filtering and drying the solids under vacuum at 55.degree. for 16 h to afford a catalyst for epoxidn. of propylene.

IT 7440-05-3, Palladium, uses 7440-06-4, Platinum, uses
(for in situ **prodn.** of hydrogen **peroxide**; use of water-treated calcined **titanium** or vanadium **zeolites** as catalysts for epoxidn. of olefins)

RN 7440-05-3 HCA

CN Palladium (8CI, 9CI) (CA INDEX NAME)

Pd

RN 7440-06-4 HCA

CN Platinum (8CI, 9CI) (CA INDEX NAME)

Pt

IT 1333-74-0, Hydrogen, reactions 7782-44-7, Oxygen, reactions

(for in situ **prodn.** of hydrogen **peroxide**; use of water-treated calcined **titanium** or vanadium **zeolites** as catalysts for epoxidn. of olefins)

RN 1333-74-0 HCA

CN Hydrogen (8CI, 9CI) (CA INDEX NAME)

H-H

RN 7782-44-7 HCA

CN Oxygen (8CI, 9CI) (CA INDEX NAME)

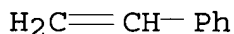
O=O

IC ICM C07D301-06

INCL 549533000; 549531000

- CC 35-2 (Chemistry of Synthetic High Polymers)
Section cross-reference(s): 27, 67
- ST water treated calcined **titanium** vanadium **zeolite**
epoxidn catalyst; hydrogen peroxide olefin epoxidn **titanium**
vanadium **zeolite** catalyst
- IT Titanium silicalite
(TS 1; use of water-treated calcined
titanium or vanadium **zeolites** as catalysts for
epoxidn. of olefins)
- IT Noble metals
(for in situ **prodn.** of hydrogen **peroxide**; use
of water-treated calcined **titanium** or vanadium
zeolites as catalysts for epoxidn. of olefins)
- IT Epoxidation
Epoxidation catalysts
(use of water-treated calcined **titanium** or vanadium
zeolites as catalysts for epoxidn. of olefins)
- IT Titanosilicate zeolites
(use of water-treated calcined **titanium** or vanadium
zeolites as catalysts for epoxidn. of olefins)
- IT Epoxides
(use of water-treated calcined **titanium** or vanadium
zeolites as catalysts for epoxidn. of olefins)
- IT Alkenes, reactions
(use of water-treated calcined **titanium** or vanadium
zeolites as catalysts for epoxidn. of olefins)
- IT Zeolites (synthetic), uses
(vanadosilicate; use of water-treated calcined **titanium**
or vanadium **zeolites** as catalysts for epoxidn. of
olefins)
- IT 7440-05-3, Palladium, uses 7440-06-4, Platinum,
uses 7440-57-5, Gold, uses
(for in situ **prodn.** of hydrogen **peroxide**; use
of water-treated calcined **titanium** or vanadium
zeolites as catalysts for epoxidn. of olefins)
- IT 1333-74-0, Hydrogen, reactions 7782-44-7, Oxygen,
reactions
(for in situ **prodn.** of hydrogen **peroxide**; use
of water-treated calcined **titanium** or vanadium
zeolites as catalysts for epoxidn. of olefins)
- IT 78-10-4, Tetraethyl orthosilicate 3087-36-3, Tetraethyl
orthotitanate
(in **prodn.** of **titanium** silicalite **zeolites**;
use of water-treated calcined **titanium** or vanadium
zeolites as catalysts for epoxidn. of olefins)
- IT 75-56-9P, Propylene oxide, preparation
(use of water-treated calcined **titanium** or vanadium
zeolites as catalysts for epoxidn. of olefins)

- IT 115-07-1, Propylene, reactions 7722-84-1, Hydrogen peroxide, reactions
(use of water-treated calcined **titanium** or vanadium **zeolites** as catalysts for epoxidn. of olefins)
- L65 ANSWER 2 OF 12 HCA COPYRIGHT 2006 ACS on STN
142:101067 Supported catalysts having a controlled coordination structure and methods for preparing such catalysts. Zhou, Bing; Rueter, Michael; Parasher, Sukesh (USA). U.S. Pat. Appl. Publ. US 2005014635 A1 20050120, 28 pp. (English). CODEN: USXXCO. APPLICATION: US 2003-618808 20030714.
- AB Supported reactive catalysts having a controlled coordination structure and methods for their prodn. are disclosed. The supported catalysts of the present invention are useful for the **prepn** . of hydrogen **peroxide** with high selectivity in addn. to other chem. conversion reactions. The supported catalyst comprises catalyst particles having top or outer layer of atoms in which at least a portion of the atoms exhibit a controlled coordination no. of 2. The catalyst and methods may be used for the concurrent in situ and ex situ conversion of org. compds. In addn., a process is provided for catalytically **producing** hydrogen **peroxide** from hydrogen and oxygen feeds by contacting them with the catalysts of the invention and a suitable org. liq. solvent having a Solvent Selection Parameter (SSP) between 0.14.times.10⁻⁴ and 5.0.times.10⁻⁴ .
- IT 100-42-5D, **Styrene**, sulfonated 7440-02-0
, **Nickel**, uses 7440-05-3, **Palladium**,
uses 7440-06-4, **Platinum**, uses
(**supported catalysts** having controlled
coordination structure and methods for prepg. such catalysts)
- RN 100-42-5 HCA
CN Benzene, ethenyl- (9CI) (CA INDEX NAME)



- RN 7440-02-0 HCA
CN Nickel (8CI, 9CI) (CA INDEX NAME)
- Ni
- RN 7440-05-3 HCA
CN Palladium (8CI, 9CI) (CA INDEX NAME)

Pd

RN 7440-06-4 HCA
CN Platinum (8CI, 9CI) (CA INDEX NAME)

Pt

IT 7782-44-7, Oxygen, uses
(supported catalysts having controlled coordination structure and
methods for prepg. such catalysts)

RN 7782-44-7 HCA
CN Oxygen (8CI, 9CI) (CA INDEX NAME)

O=O

IT 7722-84-1P, Hydrogen peroxide, preparation
(supported catalysts having controlled coordination structure and
methods for prepg. such catalysts)

RN 7722-84-1 HCA
CN Hydrogen peroxide (H2O2) (9CI) (CA INDEX NAME)

HO-OH

IT 1333-74-0, Hydrogen, reactions
(supported catalysts having controlled coordination structure and
methods for prepg. such catalysts)

RN 1333-74-0 HCA
CN Hydrogen (8CI, 9CI) (CA INDEX NAME)

H-H

IC ICM B01J031-00

INCL 502159000; 502150000; 502155000

CC 67-1 (Catalysis, Reaction Kinetics, and Inorganic Reaction
Mechanisms)

Section cross-reference(s): 49, 78

ST supported catalyst controlled coordination structure prepn; hydrogen
peroxide prodn supported catalyst controlled
coordination structure

IT Titanosilicate zeolites

(TS-1; supported catalysts having controlled
coordination structure and methods for prepg. such catalysts)

IT 100-42-5D, Styrene, sulfonated 1344-28-1,
Alumina, uses 7439-88-5, Iridium, uses 7439-89-6, Iron, uses
7439-91-0, Lanthanum, uses 7439-96-5, Manganese, uses 7439-98-7,
Molybdenum, uses 7440-02-0, Nickel, uses

7440-04-2, Osmium, uses **7440-05-3, Palladium**,
uses **7440-06-4, Platinum**, uses 7440-15-5,
Rhenium, uses 7440-16-6, Rhodium, uses 7440-18-8, Ruthenium,
uses 7440-31-5, Tin, uses 7440-32-6, Titanium, uses 7440-33-7,
Tungsten, uses 7440-44-0, Carbon, uses 7440-45-1, Cerium, uses
7440-47-3, Chromium, uses 7440-48-4, Cobalt, uses 7440-50-8,
Copper, uses 7440-57-5, Gold, uses 7440-62-2, Vanadium, uses
7440-66-6, Zinc, uses 7440-67-7, Zirconium, uses 7631-86-9,
Silica, uses 7727-37-9, Nitrogen, uses 7782-42-5, Graphite, uses
9002-89-5, Polyvinyl alcohol 9003-01-4, Polyacrylic acid
9003-01-4D, Polyacrylic acid, salts 25013-01-8, Polypyridine
25038-59-9D, sulfonated 25191-25-7, Polyvinyl sulfate
25322-68-3, Polyethylene glycol 25322-69-4, Polypropylene glycol

(**supported catalysts** having controlled
coordination structure and methods for prepg. such catalysts)

- IT **7782-44-7, Oxygen**, uses
(supported catalysts having controlled coordination structure and
methods for prepg. such catalysts)
- IT **7722-84-1P, Hydrogen peroxide, preparation**
(supported catalysts having controlled coordination structure and
methods for prepg. such catalysts)
- IT **1333-74-0, Hydrogen, reactions**
(supported catalysts having controlled coordination structure and
methods for prepg. such catalysts)

L65 ANSWER 3 OF 12 HCA COPYRIGHT 2006 ACS on STN

140:96308 Hydrogen **peroxide production** using
catalyst particles with controlled surface coordination number.
Zhou, Bing; Rueter, Michael (Hydrocarbon Technologies Inc., USA).
U.S. Pat. Appl. Publ. US 2004018143 A1 20040129, 17 pp.,
Cont.-in-part of U.S. Ser. No. 205,881, abandoned. (English).
CODEN: USXXCO. APPLICATION: US 2003-357573 20030205. PRIORITY: US
2002-2002/205881 20020726.

AB Hydrogen **peroxide** is **produced** from hydrogen and
oxygen feeds by contacting them with a supported noble metal
catalyst and a suitable org. liq. solvent having a Solvent Selection
Parameter (SSP) between 0.14.times.10⁻⁴ and 5.0.times.10⁻⁴ at
reaction condition of 30-80.degree. and 500-2500 psig pressure. The
catalyst consists of supported noble metal particles having an
exposed crystal face at. surface structure with atoms exhibiting a
controlled coordination no. of two. The nearest neighbors of each
top-layer atom are two other top-layer atoms, also having a
controlled coordination no. of two (2). The org. solvent can be
methanol, ethanol, n-propanol, isopropanol, acetone, acetonitrile,
1-propylamine, or their mixts. with water. The liq. mixt. contains
1-500 ppm by wt. NaBr promoter. The noble metals can be Pd, Pt, Ir,
Au, Os, Ru, Rh, or Re. The solid support material is a carbon based
material, such as carbon black; fluoridated carbon, or activated

carbon. The solid support material can contain other catalytic materials, such as Ti- or V-substituted silicalites; other substituted **zeolites** contg. Ti, V, Te, B, Ge, or Nb; catalysts contg. Si and Ti which are isomorphous with **zeolite** beta; **titanium** aluminophosphates; Cr and Fe incorporated silica aluminophosphates; Fe-substituted silicotungstates; zeolite **encapsulated** vanadium picolinate peroxo complexes; metal oxides including TiO₂, MoO₃, WO₃ and substituted silica xerogels; molybdenum vanadium-phosphate compds.; and Cr-contg. heteropolytungstates. The solid support material has a surface area between 50 and 500 m²/g. The supported noble metal catalyst is prepd. by forming an organometallic complex of a noble metal salt and an ionic org. polymer or chelating compd. as templating agent, depositing the organometallic complex on the surface of a solid catalyst support material, and reducing the deposited organometallic complex with H₂ to form noble metal crystals. The ionic org. polymer or chelating compd. can be cellulose succinate, polyacrylates, polyvinylbenzoates, polyvinyl sulfate, polyvinyl sulfonates, sulfonated **styrene**, polybisphenol carbonates, polybenzimidazoles, polypyridine, sulfonated polyethylene terephthalate, polyvinyl alc. acetate and succinate, polyethylene glycol, polypropylene glycol, ethylene and propylenediamine, cyclic diamines, such as piperidine, EDTA, pyromellitic acid, salicylic acid, hydroxymalonic acid, and urea.

IT 7440-05-3, Palladium, uses 7440-06-4, Platinum,
uses
(hydrogen **peroxide** prodn. using catalyst
particles with controlled surface coordination no.)

RN 7440-05-3 HCA
CN Palladium (8CI, 9CI) (CA INDEX NAME)

Pd

RN 7440-06-4 HCA
CN Platinum (8CI, 9CI) (CA INDEX NAME)

Pt

IT 7722-84-1P, Hydrogen **peroxide**, preparation
(hydrogen **peroxide** prodn. using catalyst
particles with controlled surface coordination no.)

RN 7722-84-1 HCA
CN Hydrogen peroxide (H₂O₂) (9CI) (CA INDEX NAME)

HO-OH

IT 100-42-5D, **Styrene**, sulfonated 1333-74-0
, Hydrogen, reactions 7782-44-7, Oxygen, reactions
(hydrogen **peroxide prodn.** using catalyst
particles with controlled surface coordination no.)
RN 100-42-5 HCA
CN Benzene, ethenyl- (9CI) (CA INDEX NAME)

$\text{H}_2\text{C}=\text{CH}-\text{Ph}$

RN 1333-74-0 HCA
CN Hydrogen (8CI, 9CI) (CA INDEX NAME)

$\text{H}-\text{H}$

RN 7782-44-7 HCA
CN Oxygen (8CI, 9CI) (CA INDEX NAME)

$\text{O}=\text{O}$

IC ICM C01B015-029
INCL 423584000; 502325000
CC 49-8 (Industrial Inorganic Chemicals)
Section cross-reference(s): 67
ST hydrogen **peroxide manuf** noble metal catalyst
IT Silicalites (zeolites)
(V-substituted; hydrogen **peroxide prodn.**
using catalyst particles with controlled surface coordination
no.)
IT Carbon black, uses
(catalyst support; hydrogen **peroxide prodn.**
using catalyst particles with controlled surface coordination
no.)
IT Xerogels
(hydrogen **peroxide prodn.** using catalyst
particles with controlled surface coordination no.)
IT Beta zeolites
Noble metals
Titanium silicalite
(hydrogen **peroxide prodn.** using catalyst
particles with controlled surface coordination no.)
IT Acrylic polymers, reactions
(hydrogen **peroxide prodn.** using catalyst
particles with controlled surface coordination no.)
IT Polybenzimidazoles

- (hydrogen **peroxide prodn.** using catalyst particles with controlled surface coordination no.)
- IT Polyoxyalkylenes, reactions
(hydrogen **peroxide prodn.** using catalyst particles with controlled surface coordination no.)
- IT Polyesters, reactions
(sulfonated; hydrogen **peroxide prodn.** using catalyst particles with controlled surface coordination no.)
- IT Heteropoly acids
(tungstates, Cr-contg.; hydrogen **peroxide prodn.** using catalyst particles with controlled surface coordination no.)
- IT 11121-26-9, Silicotungstate
(Fe-substituted; hydrogen **peroxide prodn.** using catalyst particles with controlled surface coordination no.)
- IT 7440-44-0, Carbon, uses
(activated or fluoridated, catalyst support; hydrogen **peroxide prodn.** using catalyst particles with controlled surface coordination no.)
- IT 1313-27-5, Molybdenum oxide (MoO₃), uses 1314-35-8, Tungsten oxide (WO₃), uses 7439-88-5, Iridium, uses 7440-04-2, Osmium, uses **7440-05-3**, Palladium, uses **7440-06-4**, Platinum, uses 7440-15-5, Rhenium, uses 7440-16-6, Rhodium, uses 7440-18-8, Ruthenium, uses 7440-57-5, Gold, uses 13463-67-7, Titanium oxide (TiO₂), uses 80927-59-9, Titanium aluminophosphate
(hydrogen **peroxide prodn.** using catalyst particles with controlled surface coordination no.)
- IT **7722-84-1P**, Hydrogen **peroxide, preparation**
(hydrogen **peroxide prodn.** using catalyst particles with controlled surface coordination no.)
- IT 57-13-6, Urea, reactions 60-00-4, EDTA, reactions 69-72-7, Salicylic acid, reactions 78-90-0, Propylenediamine 80-69-3, Hydroxymalonic acid 89-05-4, Pyromellitic acid **100-42-5D**, **Styrene**, sulfonated 107-15-3, Ethylenediamine, reactions 110-89-4, Piperidine, reactions **1333-74-0**, Hydrogen, reactions **7782-44-7**, Oxygen, reactions 9003-04-7, Sodium polyacrylate 24991-32-0D, Polyvinylbenzoate, derivs. 25013-01-8, Polypyridine 25037-45-0D, Carbonic acid, polymer with 4,4'-(1-methylethylidene)bis[phenol], salts 25038-59-9D, Polyethylene terephthalate, sulfonated 25191-25-7, Polyvinyl sulfate 25322-68-3, Polyethylene glycol 25322-69-4, Polypropylene glycol 26101-52-0D, Polyvinyl sulfonic acid, salts 53125-04-5, Polyvinyl alcohol succinate 57126-19-9, Cellulose succinate 122303-55-3, Polyvinyl alcohol acetate
(hydrogen **peroxide prodn.** using catalyst particles with controlled surface coordination no.)
- IT 7647-15-6, Sodium bromide (NaBr), uses

- (promoter; hydrogen **peroxide prodn.** using catalyst particles with controlled surface coordination no.)
- IT 64-17-5, Ethanol, uses 67-56-1, Methanol, uses 67-63-0, Isopropanol, uses 67-64-1, Acetone, uses 71-23-8, n-Propanol, uses 75-05-8, Acetonitrile, uses 107-10-8, 1-Propylamine, uses 7732-18-5, Water, uses (solvent; hydrogen **peroxide prodn.** using catalyst particles with controlled surface coordination no.)
- L65 ANSWER 4 OF 12 HCA COPYRIGHT 2006 ACS on STN
- 139:388328 Heteropolyacid-**encapsulated** TiHY zeolite as an inorganic photosynthetic reaction center mimicking the plant systems. Anandan, Sambandam; Yoon, Minjoong (Department of Chemistry, Chungnam National University, Taejeon, 305-764, S. Korea). Journal of Photochemistry and Photobiology, A: Chemistry, 160(3), 181-184 (English) 2003. CODEN: JPPCEJ. ISSN: 1010-6030. Publisher: Elsevier Science B.V..
- AB A tremendous breakthrough was required for the researchers trying to find a way to photodecompn. of water by using semiconductor photocatalysts without electricity. In this regard, we attempted to prep. the heteropolyacid (HPA)-**encapsulated** TiHY zeolite a new photocatalyst mimicking the plant photosynthetic system. This photocatalyst (0.3 g/40 mL) was obsd. to generate hydrogen (4.08.+-.0.7 .mu.l/h) and oxygen (6.86.+-.0.7 .mu.l/h) from the aq. solns. upon illumination by two photon reactions (UV and visible lights), which is quite analogous to the "Z-scheme" mechanism for plant photosynthetic systems. The turnover no. of the photocatalyst was detd. to be 11 with the quantum yield of the water splitting about 27.+-.6% at 352 nm. Thus, this inorg. material must be very useful as a reaction center mimicking the plant photosynthetic system without elec. energy.
- IT 1333-74-0, **Hydrogen, processes**
7782-44-7, **Oxygen, processes**
(heteropolyacid-**encapsulated** TiHY zeolite as photocatalyst to generate hydrogen and oxygen from aq. solns.)
- RN 1333-74-0 HCA
- CN Hydrogen (8CI, 9CI) (CA INDEX NAME)
- H-H
- RN 7782-44-7 HCA
- CN Oxygen (8CI, 9CI) (CA INDEX NAME)
- O=O
- CC 74-1 (Radiation Chemistry, Photochemistry, and Photographic and

Other Reprographic Processes)

Section cross-reference(s): 8, 11

- ST heteropolyacid **encapsulated** TiHY zeolite hydrogen prodn
water; plant photosynthetic system mimicking photocatalyst
heteropolyacid **encapsulated** TiHY zeolite
- IT Photosystems
(heteropolyacid-**encapsulated** TiHY zeolite as inorg.
photosynthetic reaction center mimicking plant photosystems)
- IT Photolysis catalysts
(heteropolyacid-**encapsulated** TiHY zeolite as
photocatalyst to generate hydrogen and oxygen from aq. solns.)
- IT **Zeolite HY**
(**titanium**-exchanged; heteropolyacid-
encapsulated TiHY zeolite as photocatalyst to generate
hydrogen and oxygen from aq. solns.)
- IT 13463-67-7, Titanium oxide (TiO₂), properties
(heteropolyacid-**encapsulated** TiHY zeolite as
photocatalyst to generate hydrogen and oxygen from aq. solns.)
- IT **1333-74-0, Hydrogen, processes**
7782-44-7, Oxygen, processes
(heteropolyacid-**encapsulated** TiHY zeolite as
photocatalyst to generate hydrogen and oxygen from aq. solns.)
- IT 1343-93-7D, reaction products
(heteropolyacid-**encapsulated** TiHY zeolite as
photocatalyst to generate hydrogen and oxygen from aq. solns.)
- IT 64-17-5, Ethanol, processes
(heteropolyacid-**encapsulated** TiHY zeolite as
photocatalyst to generate hydrogen and oxygen from aq. solns.)
- IT 7732-18-5, Water, reactions
(heteropolyacid-**encapsulated** TiHY zeolite as
photocatalyst to generate hydrogen and oxygen from aq. solns.)
- IT 1343-93-7
(heteropolyacid-**encapsulated** TiHY zeolite as
photocatalyst to generate hydrogen and oxygen from aq. solns.)

L65 ANSWER 5 OF 12 HCA COPYRIGHT 2006 ACS on STN

138:287333 Direct hydroxylation of aromatics with a mixture of
H₂ and **O₂** gases over Fe- and Pd-incorporated
zeolites. Hwang, J.-S.; Lee, C. W.; Ahn, D. H.; Chai, H. S.; Park,
S.-E. (Catalysis Center for Molecular Engineering, KRICT, Daejeon,
305-600, S. Korea). Research on Chemical Intermediates, 28(6),
527-535 (English) 2002. CODEN: RCINEE. ISSN: 0922-6168. OTHER
SOURCES: CASREACT 138:287333. Publisher: VSP BV.

AB The hydroxylation of benzene and phenol with in situ generated
oxidant was performed under mild reaction conditions over a
bicatalytic system which has dual abilities of direct **H₂O₂**
generation and hydroxylation activity by combining
Pd-zeolite with redox zeolites such as **TS-1**,

Ti-MCM-41, V-MCM-41 and Fe-zeolite. The amt. of **H2O2** **formed** directly from **H2** and **O2** increases with increasing Pd loading over zeolite up to 0.6% and subsequently decreases slightly as the Pd loading increases. The optimum amt. of **H2O2 produced** is 6.4 mmol. Over Pd/HBEA + Fe/Y, when **H2:O2** = 40:40 mL/min is supplied, phenol conversion increases from 4.6% at 2 h to 13.6% at 8 h with high catechol selectivity in the range of 65-79%. The hydroxylation activities over redox catalyst with **H2O2** are compared. Hydroxylation activity is improved by **encapsulating** FePc onto Y zeolite. In terms of TON, FePc/Y exhibits 3.5 times higher capacity than Fe/Y.

IT 7440-05-3, Palladium, uses
(direct hydroxylation of benzene and phenol with **H2-O2** mixt. over Fe- and Pd-incorporated zeolites)
RN 7440-05-3 HCA
CN Palladium (8CI, 9CI) (CA INDEX NAME)

Pd

IT 7722-84-1P, Hydrogen **peroxide**, preparation
(direct hydroxylation of benzene and phenol with **H2-O2** mixt. over Fe- and Pd-incorporated zeolites)
RN 7722-84-1 HCA
CN Hydrogen peroxide (**H2O2**) (9CI) (CA INDEX NAME)

HO-OH

CC 25-10 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
ST hydroxylation benzene phenol iron palladium zeolite; pyrocatechol
prepn iron palladium zeolite; hydroquinone prep iron palladium
zeolite; hydrogen **peroxide prep** iron palladium
zeolite
IT Hydroxylation catalysts
(direct hydroxylation of benzene and phenol with **H2-O2** mixt. over Fe- and Pd-incorporated zeolites)
IT H-Beta zeolites
Titanium silicalite
Y zeolites
Zeolite MCM-41
(direct hydroxylation of benzene and phenol with **H2-O2** mixt. over Fe- and Pd-incorporated zeolites)
IT 132-16-1, Iron phthalocyanine 7439-89-6, Iron, uses
7440-05-3, Palladium, uses 7440-32-6, Titanium, uses
7440-62-2, Vanadium, uses
(direct hydroxylation of benzene and phenol with **H2-**

- IT 71-43-2, Benzene, reactions
(direct hydroxylation of benzene and phenol with H₂-
O₂ mixt. over Fe- and Pd-incorporated zeolites)
- IT 108-95-2P, Phenol, preparation 7722-84-1P, Hydrogen
peroxide, preparation
(direct hydroxylation of benzene and phenol with H₂-
O₂ mixt. over Fe- and Pd-incorporated zeolites)
- IT 120-80-9P, Pyrocatechol, preparation 123-31-9P, Hydroquinone,
preparation
(direct hydroxylation of benzene and phenol with H₂-
O₂ mixt. over Fe- and Pd-incorporated zeolites)

L65 ANSWER 6 OF 12 HCA COPYRIGHT 2006 ACS on STN

138:239699 Integrated process and dual-function catalyst for olefin
epoxidation. Zhou, Bing; Rueter, Michael (Hydrocarbon Technologies,
Inc., USA). U.S. US 6534661 B1 20030318, 11 pp. (English). CODEN:
USXXAM. APPLICATION: US 2001-996920 20011130. PRIORITY: US
2000-PV258535 20001228.

AB The invention discloses a dual-functional catalyst compn. and an
integrated process for prodn. of olefin epoxides including propylene
oxide by catalytic reaction of hydrogen peroxide from hydrogen and
oxygen with olefin feeds such as propylene. The epoxides and
hydrogen **peroxide** are preferably **produced**
simultaneously in situ. The dual-functional catalyst comprises
noble metal crystallites with dimensions on the nanometer scale (on
the order of <1 nm to 10 nm), specially dispersed on titanium
silicalite substrate particles. The dual functional catalyst
catalyzes both the direct reaction of hydrogen and oxygen to
generate hydrogen **peroxide** intermediate on the
noble metal catalyst surface and the reaction of the hydrogen
peroxide intermediate with the propylene feed to generate propylene
oxide product. Combining both these functions in a single catalyst
provides a very efficient integrated process operable below the
flammability limits of hydrogen and highly selective for the
prodn. of hydrogen **peroxide** to **produce**
olefin oxides such as propylene oxide without formation of undesired
co-products.

IT 7722-84-1P, Hydrogen **peroxide, preparation**
(integrated process and dual-function catalyst for olefin
epoxidn.)

RN 7722-84-1 HCA

CN Hydrogen peroxide (H₂O₂) (9CI) (CA INDEX NAME)

HO-OH

IT 1333-74-0, Hydrogen, reactions 7782-44-7

, **Oxygen**, reactions

(integrated **process** and dual-function catalyst for olefin epoxidn.)

RN 1333-74-0 HCA

CN Hydrogen (8CI, 9CI) (CA INDEX NAME)

H-H

RN 7782-44-7 HCA

CN Oxygen (8CI, 9CI) (CA INDEX NAME)

O=O

IT 7440-05-3, Palladium, uses 7440-06-4, Platinum, uses

(nanometer-sized crystallites; integrated process and dual-function catalyst for olefin epoxidn.)

RN 7440-05-3 HCA

CN Palladium (8CI, 9CI) (CA INDEX NAME)

Pd

RN 7440-06-4 HCA

CN Platinum (8CI, 9CI) (CA INDEX NAME)

Pt

IC ICM B01J029-89

ICS B01J029-068; C01B015-029; C07D301-12; C07D301-03

INCL 549531000; 549532000; 549524000; 423584000; 502064000; 502066000; 502071000; 502074000; 502077000

CC 45-4 (Industrial Organic Chemicals, Leather, Fats, and Waxes)

IT **Zeolites** (synthetic), uses

(**titanium**-based; integrated process and dual-function catalyst for olefin epoxidn.)

IT 7722-84-1P, Hydrogen **peroxide**, preparation

(integrated process and dual-function catalyst for olefin epoxidn.)

IT 115-07-1, Propylene, reactions 1333-74-0, **Hydrogen**

, reactions 7782-44-7, **Oxygen**, reactions

(integrated **process** and dual-function catalyst for olefin epoxidn.)

IT 7439-88-5, Iridium, uses 7440-04-2, Osmium, uses 7440-05-3

, Palladium, uses 7440-06-4, Platinum, uses 7440-16-6,

Rhodium, uses 7440-18-8, Ruthenium, uses 7440-57-5, Gold, uses (nanometer-sized crystallites; integrated process and dual-function catalyst for olefin epoxidn.)

L65 ANSWER 7 OF 12 HCA COPYRIGHT 2006 ACS on STN

137:185988 Direct alkene epoxidation process using a catalyst comprising palladium on a niobium-containing support. Grey, Roger A. (Arco Chemical Technology, L.P., USA). U.S. US 6441203 B1 20020827, 4 pp. (English). CODEN: USXXAM. APPLICATION: US 2001-45861 20011019.

AB A liq.-phase process for epoxidizing an olefin (e.g., propylene into propylene oxide) with hydrogen and oxygen in the presence of a supported catalyst comprising palladium on a niobium-contg. (e.g., Nb2O5) support is described. The process exhibits good productivity and selectivity for olefin epoxidn. with hydrogen and oxygen, which is particularly surprising because typical palladium-contg. epoxidn. catalysts require the presence of a **titanium zeolite**.

IT **7782-44-7**, Oxygen, reactions
(in a direct alkene epoxidn. process using a catalyst comprising palladium on a niobium-contg. support)

RN 7782-44-7 HCA

CN Oxygen (8CI, 9CI) (CA INDEX NAME)

O=O

IT **1333-74-0**, Hydrogen, reactions
(in a direct alkene epoxidn. process using a catalyst comprising palladium on a niobium-contg. support)

RN 1333-74-0 HCA

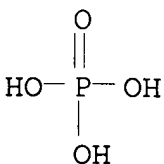
CN Hydrogen (8CI, 9CI) (CA INDEX NAME)

H-H

IT **7664-38-2**, **Phosphoric acid**, reactions
(in buffer prepn. for a direct alkene epoxidn. process using a catalyst comprising palladium on a niobium-contg. support)

RN 7664-38-2 HCA

CN Phosphoric acid (7CI, 8CI, 9CI) (CA INDEX NAME)



- IC ICM C07D301-06
INCL 549533000
CC 35-2 (Chemistry of Synthetic High Polymers)
Section cross-reference(s): 27, 48, 67
IT 7782-44-7, Oxygen, reactions
(in a direct alkene epoxidn. process using a catalyst comprising palladium on a niobium-contg. support)
IT 1333-74-0, Hydrogen, reactions
(in a direct alkene epoxidn. process using a catalyst comprising palladium on a niobium-contg. support)
IT 1310-58-3, Potassium hydroxide, reactions 7664-38-2, Phosphoric acid, reactions 7778-77-0, Potassium dihydrogen phosphate 21351-79-1, Cesium hydroxide
(in buffer prepn. for a direct alkene epoxidn. process using a catalyst comprising palladium on a niobium-contg. support)
- L65 ANSWER 8 OF 12 HCA COPYRIGHT 2006 ACS on STN
137:127083 H2O2 in CO2/H2O Biphasic Systems: Green Synthesis and Epoxidation Reactions. Hancu, Dan; Green, Jordan; Beckman, Eric J. (Chemical Engineering Department, Carnegie Mellon University, Pittsburgh, PA, 15261, USA). Industrial & Engineering Chemistry Research, 41(18), 4466-4474 (English) 2002. CODEN: IECRED. ISSN: 0888-5885. Publisher: American Chemical Society.
- AB We have explored the **generation** of hydrogen **peroxide** directly from hydrogen and oxygen using liq. CO2 as the solvent. **Producing H2O2** directly from **H2** and **O2** in the presence of a CO2-sol. **Pd catalyst** could potentially eliminate entire unit operations and reduce raw material costs significantly. Further, homogeneous reaction in liq. CO2 allows for contact between significant concns. of **O2** and **H2**, high rates of reaction, and ready recovery of the product via stripping into water. Both Pd(+2) and **Pd(0) catalysts** were explored for the reaction; our results suggest that future work should focus on the optimization of a CO2-sol. or -dispersible **Pd(0) catalyst**. Finally, we have found that CO2/H2O2/H2O mixts. are, themselves, useful reagent systems. A biphasic aq. H2O2/CO2 mixt. is an efficient epoxidizing system, where HCO4- is formed by various reactions of water, CO2, and H2O2 and transfers of oxygen to alkenes. From our results, it appears that H2O2 can react directly with CO2, producing more percarbonate ion than in situations that employ only bicarbonate as the precursor.
- IT 7440-05-3, Palladium, uses
(**synthesis** of **H2O2** directly from **H2** and **O2** in presence of **Pd catalyst** using liq. CO2 as solvent and use of aq. biphasic H2O2-CO2 system for epoxidn. reactions)
- RN 7440-05-3 HCA

CN Palladium (8CI, 9CI) (CA INDEX NAME)

Pd

IT 7722-84-1P, Hydrogen peroxide, preparation
(**synthesis** of H₂O₂ directly from H₂
and O₂ in presence of **Pd catalyst**
using liq. CO₂ as solvent and use of aq. biphasic H₂O₂-CO₂ system
for epoxidn. reactions)

RN 7722-84-1 HCA

CN Hydrogen peroxide (H₂O₂) (9CI) (CA INDEX NAME)

HO-OH

IT 1333-74-0, Hydrogen, reactions 7782-44-7, Oxygen,
reactions
(**synthesis** of H₂O₂ directly from H₂
and O₂ in presence of **Pd catalyst**
using liq. CO₂ as solvent and use of aq. biphasic H₂O₂-CO₂ system
for epoxidn. reactions)

RN 1333-74-0 HCA

CN Hydrogen (8CI, 9CI) (CA INDEX NAME)

H-H

RN 7782-44-7 HCA

CN Oxygen (8CI, 9CI) (CA INDEX NAME)

O=O

CC 49-8 (Industrial Inorganic Chemicals)

Section cross-reference(s): 27, 45, 67

ST hydrogen **peroxide synthesis** carbon dioxide liq
solvent **palladium catalyst**; epoxidn hydrogen
peroxide carbon dioxide biphasic system; cyclohexene epoxidn
hydrogen peroxide carbon dioxide biphasic system

IT Titanium silicalite

(**TS-1**, catalyst; **synthesis** of
H₂O₂ directly from H₂ and O₂ in
presence of **Pd catalyst** using liq. CO₂ as
solvent and use of aq. biphasic H₂O₂-CO₂ system for epoxidn.
reactions)

IT Epoxidation

(**synthesis** of H₂O₂ directly from H₂

- and O₂ in presence of **Pd catalyst**
using liq. CO₂ as solvent and use of aq. biphasic H₂O₂-CO₂ system
for epoxidn. reactions)
- IT 110-83-8, Cyclohexene, processes
(**synthesis** of H₂O₂ directly from H₂
and O₂ in presence of **Pd catalyst**
using liq. CO₂ as solvent and use of aq. biphasic H₂O₂-CO₂ system
for catalytic epoxidn. of)
- IT 7440-05-3, Palladium, uses 13965-03-2,
Dichlorobis(triphenylphosphine)palladium(II) 51364-51-3,
Tris(dibenzylideneacetone)dipalladium 59840-39-0 306725-79-1
408349-52-0
(**synthesis** of H₂O₂ directly from H₂
and O₂ in presence of **Pd catalyst**
using liq. CO₂ as solvent and use of aq. biphasic H₂O₂-CO₂ system
for epoxidn. reactions)
- IT 7722-84-1P, Hydrogen peroxide, preparation
(**synthesis** of H₂O₂ directly from H₂
and O₂ in presence of **Pd catalyst**
using liq. CO₂ as solvent and use of aq. biphasic H₂O₂-CO₂ system
for epoxidn. reactions)
- IT 124-38-9, Carbon dioxide, uses
(**synthesis** of H₂O₂ directly from H₂
and O₂ in presence of **Pd catalyst**
using liq. CO₂ as solvent and use of aq. biphasic H₂O₂-CO₂ system
for epoxidn. reactions)
- IT 286-20-4P, Cyclohexene oxide
(**synthesis** of H₂O₂ directly from H₂
and O₂ in presence of **Pd catalyst**
using liq. CO₂ as solvent and use of aq. biphasic H₂O₂-CO₂ system
for epoxidn. reactions)
- IT 1333-74-0, Hydrogen, reactions 7782-44-7, Oxygen,
reactions
(**synthesis** of H₂O₂ directly from H₂
and O₂ in presence of **Pd catalyst**
using liq. CO₂ as solvent and use of aq. biphasic H₂O₂-CO₂ system
for epoxidn. reactions)

L65 ANSWER 9 OF 12 HCA COPYRIGHT 2006 ACS on STN

133:213824 Nano-chemical approach in zeolite catalysis. Jang, Nak Han;
Chang, Jong-San; Lee, Chul Wee; Kim, Dae Sung; Park, Sang-Eon
(Catalysis Center for Molecular Engineering, Korea Research
Institute of Chemical Technology (KRICT), Taejon, 305-600, S.
Korea). Kongop Hwahak, 11(5), 473-478 (Korean) 2000. CODEN:
KOHWE9. ISSN: 1225-0112. Publisher: Korean Society of Industrial
and Engineering Chemistry.

AB Nano-chem. approach in zeolite catalysis was investigated. In this
study, heterogeneous catalysts for direct **prodn.** of

H2O2 from **H2** and **O2** were designed by the **encapsulation** of 2-ethylanthraquinone together with Pd nano-species on Y zeolite. Such catalysts can **produce H2O2** from **H2** and **O2** in aq. soln. and its prodn. is synergistically enhanced with the aid of the **encapsulated** 2-ethylanthraquinone in faujasite pores. The direct hydroxylation of benzene with **H2** and **O2** was performed under mild reaction condition by the bicatalyst system with considerable activity. The modification of Pd-Y with 2-ethylanthraquinone significantly improved the activity via in-situ **generation** of **H2O2** during hydroxylation in collaboration with redox zeolites. Moreover, remarkable increase in yield of phenol was achieved upon addn. of Cl⁻ in the reaction mixt. over the bicatalyst contg. Ti⁻ or V-MCM-41. The SCR of NO with methane in excess oxygen was carried out over Pd-exchanged BEA zeolites prepd. by two different methods: with or without org. template. The Pd-exchange on BEA in the presence of org. compd. was an efficient way of introducing PdO species selectively onto the external site of zeolite pore, which seemed to be responsible for the enhanced SCR activity at lower temp.

IT 1333-74-0, Hydrogen, reactions 7782-44-7, Oxygen, reactions

(nano-chem. approach in zeolite catalysis)

RN 1333-74-0 HCA

CN Hydrogen (8CI, 9CI) (CA INDEX NAME)

H-H

RN 7782-44-7 HCA

CN Oxygen (8CI, 9CI) (CA INDEX NAME)

O=O

IT 7722-84-1P, Hydrogen peroxide, preparation

(nano-chem. approach in zeolite catalysis)

RN 7722-84-1 HCA

CN Hydrogen peroxide (H2O2) (9CI) (CA INDEX NAME)

HO-OH

CC 67-1 (Catalysis, Reaction Kinetics, and Inorganic Reaction Mechanisms)

Section cross-reference(s): 59

ST nanochem approach zeolite catalysis; hydrogen peroxide prodn ethylanthraquinone Y zeolite catalyst; hydroxylation

- benzene ethylantraquinone Y zeolite catalyst; **titanium**
MCM41 **zeolite** catalyst hydroxylation benzene; vanadium
MCM41 zeolite catalyst hydroxylation benzene; SCR nitrogen oxide
methane palladium exchanged BEA zeolite catalyst; redn nitrogen
oxide methane palladium exchange BEA zeolite catalyst
- IT 71-43-2, Benzene, reactions 74-82-8, Methane, reactions
1333-74-0, Hydrogen, reactions 7782-44-7, Oxygen,
reactions 10102-43-9, Nitric oxide, reactions
(nano-chem. approach in zeolite catalysis)
- IT 7722-84-1P, Hydrogen **peroxide, preparation**
(nano-chem. approach in zeolite catalysis)
- L65 ANSWER 10 OF 12 HCA COPYRIGHT 2006 ACS on STN
132:307847 'One-pot' reactions: a contribution to environmental
protection. Hoelderich, W. F. (Department of Chemical Technology
and Heterogeneous Catalysis, RWTH Aachen, University of Technology,
Aachen, 52074, Germany). Applied Catalysis, A: General, 194-195,
487-496 (English) 2000. CODEN: ACAGE4. ISSN: 0926-860X. OTHER
SOURCES: CASREACT 132:307847. Publisher: Elsevier Science B.V..
- AB The direct oxidn. of benzene, .beta.-picoline and propylene were
carried out by 'one-pot' reactions. A steamed H-[Al]-ZSM-5 with
strong Lewis acid sites yields the best results in the oxidn. of
benzene with N2O. .beta.-Picoline can be directly oxidized with
O2 in the gas-phase to nicotinic acid in the presence of a
V2O5-impregnated TiO2 catalyst having **Bronsted**
acid sites in addn. to redox properties. Yields up to 98%
can be achieved. The propylene oxide synthesis is based on the
oxidn. of propylene by using a O2-H2 gas mixt.
over Pd/Pt-impregnated **TS-1**. Selectivities up
to 85% are obtained at conversions between 15 and 20%.
- CC 21-2 (General Organic Chemistry)
- IT Oxidation catalysts
(one-pot; HZSM-5, divanadium pentoxide-titanium dioxide, and
palladium-platinum/**TS-1** for benzene,
.beta.-picoline, and propene)
- L65 ANSWER 11 OF 12 HCA COPYRIGHT 2006 ACS on STN
131:351043 Direct hydroxylation of benzene with **H2** and
O2 over 2-ethylantraquinone **encapsulated**
Pd[0]-Y zeolite. Park, S.-E.; Yoo, J. W.; Lee, W. J.;
Chang, J.-S.; Lee, C. W. (Industrial Catalysis Research Lab., Korea
Research Institute of Chemical Technology, Taejon, 305-606, S.
Korea). Proceedings of the International Zeolite Conference, 12th,
Baltimore, July 5-10, 1998, Meeting Date 1998, Volume 2, 1253-1260.
Editor(s): Treacy, M. M. J. Materials Research Society: Warrendale,
Pa. (English) 1999. CODEN: 68DCAH.
- AB The direct hydroxylation of benzene with gaseous **H2** and
O2 was performed under mild reaction condition using a

binary catalyst system. This catalyst promotes **formation** of hydrogen **peroxide** as well as hydroxylation benzene to phenol. The modification of Pd-Y with 2-EAQ improved the hydroxylation activity significantly via in-situ **generation** of **H2O2** during hydroxylation. Moreover, remarkably increased yield of phenol was achieved upon the addn. of Cl- in the reaction mixt. in presence of a binary catalyst contg. Ti-MCM-41 or V-MCM-41. However, in the case of V-MCM-41 contg. binary catalyst, vanadyl [(V=O)2+] species were leached out during reaction and detected from the soln. by ESR.

IT **7722-84-1P, Hydrogen peroxide, preparation**
(hydroxylation of benzene with hydrogen and oxygen over
(ethyl)anthraquinone-PdY zeolite binary catalyst)
RN 7722-84-1 HCA
CN Hydrogen peroxide (H2O2) (9CI) (CA INDEX NAME)

HO-OH

CC 25-10 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
IT **Zeolite MCM-41**

(**titanium**-exchanged or vanadium-exchanged;
hydroxylation of benzene with hydrogen and oxygen over
(ethyl)anthraquinone-PdY zeolite binary catalyst)

IT **7722-84-1P, Hydrogen peroxide, preparation**
(hydroxylation of benzene with hydrogen and oxygen over
(ethyl)anthraquinone-PdY zeolite binary catalyst)

L65 ANSWER 12 OF 12 HCA COPYRIGHT 2006 ACS on STN
124:145879 Integrated process for epoxide production involving
autoxidation of alkylammonium anthrahydroquinonesulfonate coupled
with alkene epoxidation. Rodriguez, Carmen L.; Zajacek, John G.
(Arco Chemical Technology, L.P., USA). U.S. US 5463090 A 19951031,
9 pp. (English). CODEN: USXXAM. APPLICATION: US 1994-330057
19941027.

AB Epoxides are produced by an integrated **process** involving
mol. **oxygen** oxidn. of an alkylammonium salt of a sulfonic
acid-substituted anthrahydroquinone, epoxidn. of an ethylenically
unsatd. substrate using the hydrogen **peroxide**-contg.
product obtained by such oxidn. in the presence of a
titanium silicalite catalyst, and regeneration of the
anthrahydroquinone by **hydrogenation** of the anthraquinone
co-product. Oxidn. and epoxidn. may be performed concurrently. The
alkylammonium salts have the advantage of being highly sol. in polar
protic media such as water and lower alcs.

IT **7440-02-0, Nickel**, uses **7440-05-3**,
Palladium, uses **7440-06-4**, **Platinum**,
uses

(**hydrogenation catalyst**; integrated process
for epoxide prodn. involving autoxidn. of alkylammonium
anthrahydroquinonesulfonate coupled with alkene epoxidn.)

RN 7440-02-0 HCA

CN Nickel (8CI, 9CI) (CA INDEX NAME)

Ni

RN 7440-05-3 HCA

CN Palladium (8CI, 9CI) (CA INDEX NAME)

Pd

RN 7440-06-4 HCA

CN Platinum (8CI, 9CI) (CA INDEX NAME)

Pt

IT **7722-84-1P, Hydrogen peroxide, preparation**
(in situ **formation**; integrated process for epoxide
prodn. involving autoxidn. of alkylammonium
anthrahydroquinonesulfonate coupled with alkene epoxidn.)

RN 7722-84-1 HCA

CN Hydrogen peroxide (H2O2) (9CI) (CA INDEX NAME)

HO-OH

IC ICM C07D301-12

ICS C07D303-04

INCL 549531000

CC 27-2 (Heterocyclic Compounds (One Hetero Atom))

Section cross-reference(s): 35, 45

ST epoxide prepn; autoxidn ammonium anthrahydroquinonesulfonate
integrated alkene epoxidn; titanium silicalite catalyst alkene
epoxidn; hydrogen **peroxide** in situ **formation**
epoxidn

IT Redox reaction

(alkylammonium anthrahydroquinonesulfonate
autoxidn./anthraquinonesulfonate **hydrogenation**;
integrated process for epoxide prodn. involving autoxidn. of
alkylammonium anthrahydroquinonesulfonate coupled with alkene
epoxidn.)

IT Epoxidation

Epoxidation catalysts

Hydrogenation**Hydrogenation catalysts**

Oxidation, aut-

(integrated process for epoxide prodn. involving autoxidn. of alkylammonium anthrahydroquinonesulfonate coupled with alkene epoxidn.)

IT **Zeolites**, uses

(titanium silicalite, epoxidn. catalysts; integrated process for epoxide prodn. involving autoxidn. of alkylammonium anthrahydroquinonesulfonate coupled with alkene epoxidn.)

IT **7440-02-0, Nickel**, uses **7440-05-3,****Palladium**, uses **7440-06-4, Platinum,**uses **7440-16-6, Rhodium**, uses **7440-18-8, Ruthenium**, uses **7440-47-3, Chromium**, uses**(hydrogenation catalyst; integrated process for epoxide prodn. involving autoxidn. of alkylammonium anthrahydroquinonesulfonate coupled with alkene epoxidn.)**IT **7722-84-1P, Hydrogen peroxide, preparation**

(in situ formation; integrated process for epoxide prodn. involving autoxidn. of alkylammonium anthrahydroquinonesulfonate coupled with alkene epoxidn.)

=> d his 168-

FILE 'REGISTRY'

E MCM-41/CN

L68 1 S E2

FILE 'HCA'

L69 1198 S L68 OR (TI OR TITANIUM#) (2A)MCM OR TITANOSILICATE# (2A) (

L70 44 S L69 AND L20 AND L21

L71 16 S L70 AND (L29 OR L32)

L72 3 S L71 NOT (L65 OR L66 OR L67)

=> d 172 1-3 cbib abs hitstr hitind

L72 ANSWER 1 OF 3 HCA COPYRIGHT 2006 ACS on STN

141:158948 Integrated process for selective oxidation of organic compounds. De Frutos, Pilar; Padilla, Ana; Riesco, Jose Manuel; Campos Martin, Jose Miguel; Brieva Gema, Blanco; Serrano Encarnacion, Cano; Capel Sanchez, Maria del Carmen; Garcia Fierro, Jose Luis (Repsol Quimica S.A., Spain). Eur. Pat. Appl. EP 1443020 A1 20040804, 13 pp. DESIGNATED STATES: R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK,

CY, AL, TR, BG, CZ, EE, HU, SK. (English). CODEN: EPXXDW.
APPLICATION: EP 2003-380019 20030203.

AB Oxidized compds. are produced in a continuous integrated process in liq. phase, which comprises the synthesis of non acidic **hydrogen peroxide** solns. by direct reaction between hydrogen and oxygen by catalytic reaction utilizing a noble metal catalyst, followed by direct mixing of this **hydrogen peroxide** soln. with an org. substrate, a suitable catalyst and optionally a solvent. The integrated process requires no treatment step and is particularly well adapted to the prodn. of propylene oxide.

IT 7722-84-1P, **Hydrogen peroxide**,
preparation
(integrated process for selective oxidn. of org. compds.)

RN 7722-84-1 HCA

CN Hydrogen peroxide (H2O2) (9CI) (CA INDEX NAME)

HO-OH

IT 1333-74-0, **Hydrogen**, reactions 7782-44-7
, **Oxygen**, reactions
(integrated **process** for selective oxidn. of org.
compds.)

RN 1333-74-0 HCA

CN Hydrogen (8CI, 9CI) (CA INDEX NAME)

H-H

RN 7782-44-7 HCA

CN Oxygen (8CI, 9CI) (CA INDEX NAME)

O=O

IC ICM C01B015-029
ICS C07B033-00; B01J031-10; B01J023-44; B01J023-42; C07D301-12;
C07D303-14

CC 45-4 (Industrial Organic Chemicals, Leather, Fats, and Waxes)
Section cross-reference(s): 49

ST selective oxidn org compd **hydrogen peroxide**
manuf

IT **Titanosilicate zeolites**
(MCM-41; integrated process for selective oxidn. of org. compds.)

IT **Zeolite MCM-41**
(**titanosilicate**; integrated process for selective
oxidn. of org. compds.)

- IT 7722-84-1P, **Hydrogen peroxide**,
preparation
(integrated process for selective oxidn. of org. compds.)
- IT 71-43-2, Benzene, reactions 75-65-0, 2-Methyl-2-propanol,
reactions 107-05-1, Allyl chloride 107-18-6, Allyl alcohol,
reactions 108-94-1, Cyclohexanone, reactions 108-95-2, Phenol,
reactions 110-83-8, Cyclohexene, reactions 111-66-0, 1-Octene
115-07-1, Propylene, reactions **1333-74-0, Hydrogen**
, reactions 3375-31-3, Palladium(II) acetate 7664-41-7, Ammonia,
reactions **7782-44-7, Oxygen**, reactions
10035-10-6, Hydrogen bromide, reactions
(integrated **process** for selective oxidn. of org.
compds.)
- L72 ANSWER 2 OF 3 HCA COPYRIGHT 2006 ACS on STN
- 138:56396 Process and catalysts for an integrated **hydrogen peroxide** production for use in organic-compound oxidations. Zhou, Bing; Rueter, Michael (Hydrocarbon Technologies, Inc., USA). U.S. US 6500969 B1 20021231, 10 pp., Cont.-in-part of U. S. Ser. No. 733,154. (English). CODEN: USXXAM. APPLICATION: US 2001-14068 20011211. PRIORITY: US 2000-2000/733154 20001208.
- AB A process for producing oxidized org. chem. products (e.g., propylene oxide) from various org. chem. feedstocks (e.g., propylene) utilizing as the oxidant **hydrogen peroxide** which is produced by noble metal nanocatalysis (e.g., Pd/C with titanium silicalite) with high selectivity at low hydrogen concns., from **O2** and **H2**, is described. The oxidn. process step can optionally be carried out in situ concurrent with the prodn. of **hydrogen peroxide** or in a two-stage process. In the two-stage **process**, the **hydrogen peroxide** intermediate is directly produced by noble metal nanocatalysis from hydrogen and oxygen feeds plus a suitable solvent (e.g., methanol) in a first catalytic reaction step. An org. chem. feedstock and the **hydrogen peroxide** intermediate and solvent soln. are fed into a second catalytic reactor to produce an oxidized org. chem. product; process flow diagrams are presented.
- IT 7722-84-1P, **Hydrogen peroxide**,
preparation
(**process** and catalysts for an integrated
hydrogen peroxide prodn. for use in org.-compd.
oxidns. using)
- RN 7722-84-1 HCA
- CN Hydrogen peroxide (H2O2) (9CI) (CA INDEX NAME)

IT 1333-74-0, **Hydrogen**, reactions 7782-44-7
, **Oxygen**, reactions
(**process** and catalysts for an integrated
hydrogen peroxide prodn. for use in org.-compd.
oxidns. using)
RN 1333-74-0 HCA
CN Hydrogen (8CI, 9CI) (CA INDEX NAME)

H-H

RN 7782-44-7 HCA
CN Oxygen (8CI, 9CI) (CA INDEX NAME)

O=O

IC ICM C07D301-12
ICS C07D301-06
INCL 549531000; 549518000; 549523000
CC 35-2 (Chemistry of Synthetic High Polymers)
Section cross-reference(s): 27, 48, 67
ST propylene oxide manuf propene epoxidn noble metal nanocatalyst;
oxidn org substrate **hydrogen peroxide** generation
noble metal nanocatalyst; methyloxirane manuf **hydrogen**
peroxide generation noble metal nanocatalyst
IT Platinum-group metals
Silicoaluminophosphate zeolites
Titanosilicate zeolites
(catalysts for an integrated **hydrogen peroxide**
prodn. for use in org.-compd. oxidns.)
IT Titanium silicalite
(catalysts for an integrated **hydrogen peroxide**
prodn. for use in org.-compd. oxidns. using)
IT Organic compounds, reactions
(hydrazo; **process** and catalysts for an integrated
hydrogen peroxide prodn. for use in org.-compd.
oxidns.)
IT Epoxidation catalysts
Oxidation catalysts
(noble metal nanocatalysts for an integrated **hydrogen**
peroxide prodn. for use in org.-compd. oxidns.)
IT Heterocyclic compounds
(**oxygen**; **process** and catalysts for an
integrated **hydrogen peroxide** prodn. for use
in org.-compd. oxidns.)
IT Epoxidation
Oxidation

- (process and catalysts for an integrated **hydrogen peroxide** prodn. for use in org.-compd. oxidns.)
- IT Ketones, preparation
(process and catalysts for an integrated **hydrogen peroxide** prodn. for use in org.-compd. oxidns.)
- IT Aldehydes, preparation
Carbonyl compounds (organic), preparation
(process and catalysts for an integrated **hydrogen peroxide** prodn. for use in org.-compd. oxidns.)
- IT Carboxylic acids, preparation
(process and catalysts for an integrated **hydrogen peroxide** prodn. for use in org.-compd. oxidns.)
- IT Esters, uses
(process and catalysts for an integrated **hydrogen peroxide** prodn. for use in org.-compd. oxidns.)
- IT Alcohols, reactions
Alkanes, reactions
Alkenes, reactions
Amines, reactions
Aromatic compounds
(process and catalysts for an integrated **hydrogen peroxide** prodn. for use in org.-compd. oxidns.)
- IT Carbohydrates, reactions
Fatty acids, reactions
Sulfides, reactions
(process and catalysts for an integrated **hydrogen peroxide** prodn. for use in org.-compd. oxidns.)
- IT Amine oxides
Epoxides
Phenols, preparation
Sulfoxides
(process and catalysts for an integrated **hydrogen peroxide** prodn. for use in org.-compd. oxidns. such as the manuf. of)
- IT Heterocyclic compounds
(sulfur; process and catalysts for an integrated **hydrogen peroxide** prodn. for use in org.-compd. oxidns.)
- IT Heteropoly acids
(tungstates; catalysts for an integrated **hydrogen peroxide** prodn. for use in org.-compd. oxidns.)
- IT Alcohols, reactions
Polymers, reactions
(unsatd.; process and catalysts for an integrated **hydrogen peroxide** prodn. for use in org.-compd. oxidns.)
- IT 7440-44-0, Activated carbon, uses
(activated, support; catalysts for an integrated **hydrogen peroxide** prodn. for use in org.-compd. oxidns. using)

- IT 80927-59-9, Titanium aluminophosphate
(catalysts for an integrated **hydrogen peroxide**
prodn. for use in org.-compd. oxidns.)
- IT 1313-27-5, Molybdenum trioxide, uses 1314-35-8, Tungsten trioxide,
uses 7439-88-5, Iridium, uses 7440-03-1, Niobium, uses
7440-04-2, Osmium, uses 7440-05-3, Palladium, uses 7440-06-4,
Platinum, uses 7440-16-6, Rhodium, uses 7440-18-8, Ruthenium,
uses 7440-21-3, Silicon, uses 7440-32-6, Titanium, uses
7440-42-8, Boron, uses 7440-56-4, Germanium, uses 7440-57-5,
Gold, uses 7440-66-6, Zinc, uses 13463-67-7, Titania, uses
13494-80-9, Tellurium, uses 70197-13-6, Methyl trioxorhenium
(catalysts for an integrated **hydrogen peroxide**
prodn. for use in org.-compd. oxidns. using)
- IT 75-56-9P, Methyloxirane, preparation
(process and catalysts for an integrated **hydrogen**
peroxide prodn. for use in org.-compd. oxidns.)
- IT 7722-84-1P, **Hydrogen peroxide**,
preparation
(**process** and catalysts for an integrated
hydrogen peroxide prodn. for use in org.-compd.
oxidns. using)
- IT 115-07-1, Propylene, reactions
(process and catalysts for an integrated **hydrogen**
peroxide prodn. for use in org.-compd. oxidns. using)
- IT 1333-74-0, **Hydrogen**, reactions 7782-44-7
, **Oxygen**, reactions
(**process** and catalysts for an integrated
hydrogen peroxide prodn. for use in org.-compd.
oxidns. using)
- IT 7732-18-5, Water, uses
(solvent; process and catalysts for an integrated
hydrogen peroxide prodn. for use in org.-compd.
oxidns. using)

L72 ANSWER 3 OF 3 HCA COPYRIGHT 2006 ACS on STN

127:207685 Metal-microcrystalline silica molecular sieve compositions,
and method for oxidizing a substrate using the molecular sieve and
an oxidant. Balkus, Kenneth J., Jr.; Gabrielov, Alexi G. (Board of
Regents, University of Texas System, USA; Balkus, Kenneth J., Jr.;
Gabrielov, Alexi G.). PCT Int. Appl. WO 9729046 A1 19970814, 54 pp.
DESIGNATED STATES: W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA,
CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IL, IS, JP, KE, KG,
KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO,
NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TR, TT, UA, UG, US,
UZ, VN, YU, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ,
CF, CG, CH, CI, CM, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC,
ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2.
APPLICATION: WO 1997-US1980 19970206. PRIORITY: US 1996-599536

19960206.

AB The mol. sieve compns. comprise a high-SiO₂ zeolite (UTD-1) having parallel channels having nominal pore diam. .gtorsim.7.2 .ANG. and a metal incorporated in the framework causing the compns. to function as a catalyst. The mol. sieves contain bis(pentamethylcyclopentadienyl)cobalt(III) hydroxide as guest mol. Preferably the metal incorporated in the framework is Ti. Calcined Ti-UTD-1 contg. cobalt oxide and the cobalt free mol. sieves is used as catalyst for oxidizing alkanes with H₂O₂ and t-Bu hydroperoxide, and for the room-temp. oxidn. of cyclohexane to adipic acid.

IT **7722-84-1, Hydrogen peroxide, processes 7782-44-7, Oxygen, processes**

(oxidant; high-silica zeolites for oxidizing org. substances with)

RN 7722-84-1 HCA

CN Hydrogen peroxide (H₂O₂) (9CI) (CA INDEX NAME)

HO-OH

RN 7782-44-7 HCA

CN Oxygen (8CI, 9CI) (CA INDEX NAME)

O=O

IC ICM C01B039-04

ICS C01B039-06; C01B039-08; C01B039-12; C01B039-48; C07C029-00

CC 49-5 (Industrial Inorganic Chemicals)

ST UTD silica zeolite oxidn catalyst; pentamethylcyclopentadienyl cobalt hydroxide zeolite; **titanosilicate zeolite** oxidn catalyst; alkane oxidn **hydrogen peroxide**

IT Borosilicate zeolites

Titanosilicate zeolites

(silica-high; for oxidizing org. substances with an oxidant)

IT 75-91-2, Tert-Butyl hydroperoxide **7722-84-1,**

Hydrogen peroxide, processes

7782-44-7, Oxygen, processes

(oxidant; high-silica zeolites for oxidizing org. substances with)

=> d l66 1-16 cbib abs hitstr hitind

L66 ANSWER 1 OF 16 HCA COPYRIGHT 2006 ACS on STN

144:41500 Comparison of the Catalytic Activity of Au₃, Au₄⁺, Au₅, and

Au5- in the Gas-Phase Reaction of **H2** and **O2** to **Form Hydrogen Peroxide**: A Density Functional Theory Investigation. Joshi, Ajay M.; Delgass, W. Nicholas; Thomson, Kendall T. (School of Chemical Engineering, Purdue University, West Lafayette, IN, 47907, USA). Journal of Physical Chemistry B, 109(47), 22392-22406 (English) 2005. CODEN: JPCBFK. ISSN: 1520-6106. Publisher: American Chemical Society.

AB We report a detailed d. functional theory (B3LYP) anal. of the gas-phase **H2O2** formation from **H2** and **O2** on Au3, Au4+, Au5, and Au5-. We find that **H2**, which interacts only weakly with the Au clusters, is dissociatively added across the Au-O bond, upon interaction with AunO2. One H atom is captured by the adsorbed **O2** to form the hydroperoxy intermediate (OOH), while the other H atom is captured by the Au atom. Once formed, the hydroperoxy intermediate acts as a precursor for the closed-loop catalytic cycle. An important common feature of all the pathways is that the rate-detg. step of the catalytic cycle is the second **H2** addn. to form **H2O2**. The **H2O2** desorption is followed by **O2** addn. to AunH2 to form the hydroperoxy intermediate, thus leading to the closure of the cycle. On the basis of the Gibbs free energy of activation, out of these four clusters, Au4+ is most active for the formation of the **H2O2**. The 0 K electronic energy of activation and the .DELTA.Gact at the std. conditions are 12.6 and 16.6 kcal/mol resp. The natural bond orbital charge anal. suggests that the Au clusters remain pos. charged (oxidic) in almost all the stages of the cycle. This is interesting in the context of the recent exptl. evidence for the activity of cationic Au in CO oxidn. and water-gas shift catalysts. We have also found preliminary evidence for a correlation between the activation barrier for the first **H2** addn. and the **O2** binding energy on the Au cluster. It suggests that the min. activation barrier for the first **H2** addn. is expected for the Au clusters with 7.0-9.0 kcal/mol **O2** binding energy, i.e., in the midrange of the expected interaction energy. This represents a balance between more favorable **H2** disson. when the Aun-**O2** interaction is weaker and high **O2** coverage when the interaction is stronger. On the basis of this work, we predict that the hydroperoxy intermediate formation can be both thermodynamically and kinetically viable only in a narrow range of the **O2** binding energy (10.0-12.0 kcal/mol)-a useful est. for computationally screening Au-cluster-based catalysts. We also show that a competitive channel for the OOH desorption exists. Thus, in propylene epoxidn. both OOH radicals and **H2O2** can attack the active Ti in/on the Au/TS-1 and generate the Ti-OOH sites, which can convert propylene to propylene oxide.

IT 1333-74-0, Hydrogen, reactions 7782-44-7, Oxygen, reactions

(comparison of catalytic activity of Au₃, Au₄⁺, Au₅, and Au₅⁻ in gas-phase reaction of H₂ and O₂ to form hydrogen peroxide and d. functional theory investigation)

RN 1333-74-0 HCA
CN Hydrogen (8CI, 9CI) (CA INDEX NAME)

H-H

RN 7782-44-7 HCA
CN Oxygen (8CI, 9CI) (CA INDEX NAME)

O=O

CC 67-3 (Catalysis, Reaction Kinetics, and Inorganic Reaction Mechanisms)
Section cross-reference(s): 65, 66

ST gold neutral ion cluster catalyst reaction hydrogen oxygen gasphase; hydrogen peroxide formation catalysis gold neutral ion cluster DFT

IT Density functional theory
((B3LYP; comparison of catalytic activity of Au₃, Au₄⁺, Au₅, and Au₅⁻ in gas-phase reaction of H₂ and O₂ to form hydrogen peroxide and d. functional theory investigation)

IT Molecular structure determination methods
(calcn.; comparison of catalytic activity of Au₃, Au₄⁺, Au₅, and Au₅⁻ in gas-phase reaction of H₂ and O₂ to form hydrogen peroxide and d. functional theory investigation)

IT Activation energy
Adsorbed substances
Cluster ions
Desorption
Dissociation
Free energy
Free energy of activation
Potential barrier
Potential energy
Reaction enthalpy
Transition state structure
(comparison of catalytic activity of Au₃, Au₄⁺, Au₅, and Au₅⁻ in gas-phase reaction of H₂ and O₂ to form hydrogen peroxide and d. functional theory investigation)

IT Intermediates

(comparison of catalytic activity of Au₃, Au₄⁺, Au₅, and Au₅⁻ in gas-phase reaction of H₂ and O₂ to form hydrogen peroxide and d. functional theory investigation)

IT Clusters

(metal; comparison of catalytic activity of Au₃, Au₄⁺, Au₅, and Au₅⁻ in gas-phase reaction of H₂ and O₂ to form hydrogen peroxide and d. functional theory investigation)

IT 75024-07-6, uses 105082-12-0, uses 845664-72-4, uses 860027-68-5, uses

(comparison of catalytic activity of Au₃, Au₄⁺, Au₅, and Au₅⁻ in gas-phase reaction of H₂ and O₂ to form hydrogen peroxide and d. functional theory investigation)

IT 7722-84-1, Hydrogen peroxide, properties

(comparison of catalytic activity of Au₃, Au₄⁺, Au₅, and Au₅⁻ in gas-phase reaction of H₂ and O₂ to form hydrogen peroxide and d. functional theory investigation)

IT 1333-74-0, Hydrogen, reactions 7782-44-7, Oxygen, reactions

(comparison of catalytic activity of Au₃, Au₄⁺, Au₅, and Au₅⁻ in gas-phase reaction of H₂ and O₂ to form hydrogen peroxide and d. functional theory investigation)

L66 ANSWER 2 OF 16 HCA COPYRIGHT 2006 ACS on STN

143:153876 Method and device for epoxidation of propylene using plasma of hydrogen and oxygen. Guo, Hongchen (Dalian University of Technology, Peop. Rep. China). Faming Zhuanli Shenqing Gongkai Shuomingshu CN 1546479 A 20041117, No pp. given (Chinese). CODEN: CNXXEV. APPLICATION: CN 2010-105211 20031128.

AB Hydrogen and oxygen react in a plasma generating app. of medium barrier discharging at ambient temp. and atm. to give hydrogen peroxide, which is gathered with methanol and used directly in the epoxidn. of propylene. The plasma generation app. is a coaxial sleeved glass structure and the circulation cooling water in the annular space of the sleeve also acts as an earth electrode. The epoxidn. of propylene is carried out in batch or fixed bed reactor with titanium-contg. zeolite as the catalyst.

IT 1333-74-0, Hydrogen, reactions 7782-44-7, Oxygen, reactions

(epoxidn. of propylene using plasma of hydrogen and oxygen in presence of titanium-contg. zeolite catalysts)

RN 1333-74-0 HCA

CN Hydrogen (8CI, 9CI) (CA INDEX NAME)

H-H

RN 7782-44-7 HCA

CN Oxygen (8CI, 9CI) (CA INDEX NAME)

O=O

IC ICM C07D305-04

CC 35-2 (Chemistry of Synthetic High Polymers)

ST epoxidn propylene plasma hydrogen oxygen; **titanium zeolite** catalyst epoxidn propylene

IT Titanium silicalite

(**TS-1** and **TS-2**; epoxidn. of propylene using plasma of hydrogen and oxygen in presence of **titanium** -contg. **zeolite** catalysts)

IT Epoxidation

Epoxidation catalysts

Plasma

(epoxidn. of propylene using plasma of hydrogen and oxygen in presence of **titanium**-contg. **zeolite** catalysts)

IT Beta **zeolites**

(**titanium**-contg.; epoxidn. of propylene using plasma of hydrogen and oxygen in presence of **titanium**-contg. **zeolite** catalysts)

IT 7440-32-6, Titanium, uses

(epoxidn. of propylene using plasma of hydrogen and oxygen in presence of **titanium**-contg. **zeolite** catalysts)

IT 75-56-9P, Propylene oxide, preparation

(epoxidn. of propylene using plasma of hydrogen and oxygen in presence of **titanium**-contg. **zeolite** catalysts)

IT 115-07-1, Propylene, reactions

(epoxidn. of propylene using plasma of hydrogen and oxygen in presence of **titanium**-contg. **zeolite** catalysts)

IT 1333-74-0, Hydrogen, reactions 7782-44-7, Oxygen, reactions

(epoxidn. of propylene using plasma of hydrogen and oxygen in presence of **titanium**-contg. **zeolite** catalysts)

- 142:413296 Manufacture of cyclohexanone oxime combined with anthraquinone **process** for **hydrogen peroxide production**. Wang, Yaquan; Liu, Tengfei; Mi, Zhentao (Tianjin University, Peop. Rep. China). Faming Zhuanli Shengqing Gongkai Shuomingshu CN 1472197 A 20040204, 6 pp. (Chinese). CODEN: CNXXEV. APPLICATION: CN 2003-129996 20030606.
- AB The cyclohexanone oxime is prepd. by the combination of the following processes: (a) anthraquinone **process** for **hydrogen peroxide prodn.**; and (b) cyclohexanone ammoxidn. with **hydrogen peroxide**. The anthraquinone process comprises the following steps: **hydrogenating** anthraquinone in C9 arene (60-80 wt%) -trioctyl phosphate (20-40 wt%) in the presence of palladium-based (0.1-0.3 wt%) catalyst at 30-80.degree. and 0.1-0.3 MPa; oxidizing with **air** or **O2** at 40-50.degree. and 0.15-0.30 MPa to obtain **hydrogen peroxide**-contg. work soln.; and extg. with 20-50% **methanol**-water soln. (extractant recovered from ammonia distn. tower) to obtain 8-30 wt% **hydrogen peroxide** soln.;. The cyclohexanone ammoxidn. process comprises the following steps: ammoxidizing cyclohexanone with the **hydrogen peroxide** soln. (at a molar ratio of 1:1-1.2 to cyclohexanone) and NH3 (at a molar ratio of 1:1.2-2.2 to cyclohexanone) in the presence of Ti-Si mol. sieve **TS-1** (1.0-2.0 wt%) as catalyst at 50-80.degree. and normal or higher pressure to obtain cyclohexanone oxime soln.; and distg. to recover un-reacted NH3. The advantage of this design is that extd. **hydrogen peroxide** is directly injected into the cyclohexanone oximation chamber, and the extractant (**methanol**-water solvent) recovered from ammonia distn. tower goes back to the extg. tower for **hydrogen peroxide** extn. Thus, the process reduces cost of cyclohexanone oxime manuf. and avoids the generation of pollutant.
- IT **7722-84-1P, Hydrogen peroxide, preparation**
(manuf. of cyclohexanone oxime combined with anthraquinone **process** for **hydrogen peroxide prodn.**)
- RN 7722-84-1 HCA
- CN Hydrogen peroxide (H2O2) (9CI) (CA INDEX NAME)
- HO-OH
- IC ICM C07C255-44
ICS C07C249-04
- CC 45-4 (Industrial Organic Chemicals, Leather, Fats, and Waxes)
- ST anthraquinone **process hydrogen peroxide prodn**; cyclohexanone ammoxidn cyclohexanone oxime

- IT Aromatic hydrocarbons, uses
(C9; manuf. of cyclohexanone oxime combined with anthraquinone
**process for hydrogen peroxide
prodn.**)
- IT Titanium silicalite
(ammoxidn. catalyst; manuf. of cyclohexanone oxime combined with
anthraquinone **process for hydrogen
peroxide prodn.**)
- IT 100-64-1P
(manuf. of cyclohexanone oxime combined with anthraquinone
**process for hydrogen peroxide
prodn.**)
- IT 7722-84-1P, Hydrogen peroxide,
preparation
(manuf. of cyclohexanone oxime combined with
anthraquinone **process for hydrogen
peroxide prodn.**)
- IT 78-42-2, Trioctyl phosphate
(manuf. of cyclohexanone oxime combined with anthraquinone
**process for hydrogen peroxide
prodn.**)
- IT 108-94-1, Cyclohexanone, reactions 7664-41-7, Ammonia, reactions
(manuf. of cyclohexanone oxime combined with anthraquinone
**process for hydrogen peroxide
prodn.**)
- IT 84-65-1, Anthraquinone
(manuf. of cyclohexanone oxime combined with anthraquinone
**process for hydrogen peroxide
prodn.**)

L66 ANSWER 4 OF 16 HCA COPYRIGHT 2006 ACS on STN

- 142:156346 Propylene oxidation to propylene oxide over Ag/TS-
1 catalyst in the gas phase. Wang, Rui-pu; Hao, Jing-quan;
Guo, Xin-wen; Wang, Xiang-sheng; Liu, Xue-wu (State Key Laboratory
of Fine Chemicals, Dalian University of Technology, Dalian, 116012,
Peop. Rep. China). Shiyou Xuebao, Shiyou Jiagong, 20(4), 44-50
(Chinese) 2004. CODEN: SXSHEY. ISSN: 1001-8719. Publisher: Shiyou
Xuebao, Shiyou Jiagong Bianjibu.
- AB Synthesis of propylene oxide through gas phase epoxidn. of propylene
using mol. oxygen as an oxidant over lab-prepd. Ag/TS-
1 catalyst and the lab fixed-bed reaction unit with quartz
reactor was studied. The prepn. conditions of Ag/TS-
1 catalyst such as, Ag loading, type of support, the Si/Ti
mol ratio of TS-1, calcination conditions, etc.
were investigated. The effects of reaction conditions including
reaction temp., gas velocity, vol. ratio of C₃H₆/O₂ and
C₃H₆/H₂ on catalyst performance were also investigated.
The optimum Ag loading w(Ag) was of 2% (mass percent) and

n(Si)/n(Ti) was of 64 (support), and the optimum calcination temp. was 450.degree.C in **air** for Ag/TS-1 catalyst. The reaction when carried out at 150.degree.C by passing the reactant mixt. of C₃H₆, O₂, H₂ and N₂ through the reactor at a vol. ratio of 1:2:3:12 with a space velocity of 4000 h⁻¹ is optimum. After 70 min reaction, propylene conversion (x(C₃H₆)) and selectivity to propylene oxide (SPO) were 1.37% and 93.51%, resp.

IT 1333-74-0, **Hydrogen**, uses
(calcination atm. effect on propylene oxidn. to propylene oxide over Ag/TS-1 catalyst in gas phase)

RN 1333-74-0 HCA

CN Hydrogen (8CI, 9CI) (CA INDEX NAME)

H-H

IT 7722-84-1, **Hydrogen peroxide**, reactions
7782-44-7, **Oxygen**, reactions
(oxidant; propylene oxidn. to propylene oxide over Ag/TS-1 catalyst in gas phase)

RN 7722-84-1 HCA

CN Hydrogen peroxide (H₂O₂) (9CI) (CA INDEX NAME)

HO-OH

RN 7782-44-7 HCA

CN Oxygen (8CI, 9CI) (CA INDEX NAME)

O=O

IT 124-38-9P, **Carbon dioxide**, preparation
(propylene oxidn. to propylene oxide over Ag/TS-1 catalyst in gas phase)

RN 124-38-9 HCA

CN Carbon dioxide (8CI, 9CI) (CA INDEX NAME)

O=C=O

CC 35-2 (Chemistry of Synthetic High Polymers)
Section cross-reference(s): 45, 67

IT **Air**
(calcination atm. effect on propylene oxidn. to propylene oxide over Ag/TS-1 catalyst in gas phase)

- IT Zeolite HZSM-5
(catalyst support effect on propylene oxidn. to propylene oxide over Ag/TS-1 catalyst in gas phase)
- IT Titanium silicalite
(catalyst support; propylene oxidn. to propylene oxide over Ag/TS-1 catalyst in gas phase)
- IT Calcination
Controlled atmospheres
Particle size
(effect on propylene oxidn. to propylene oxide over Ag/TS-1 catalyst in gas phase)
- IT Catalyst supports
Oxidation catalysts
(oxidn. catalyst supports; effect on propylene oxidn. to propylene oxide over Ag/TS-1 catalyst in gas phase)
- IT Chemoselectivity
Epoxidation
Epoxidation catalysts
(propylene oxidn. to propylene oxide over Ag/TS-1 catalyst in gas phase)
- IT Aldehydes, preparation
(propylene oxidn. to propylene oxide over Ag/TS-1 catalyst in gas phase)
- IT Silicalites (zeolites)
(silicalite 1; catalyst support effect on propylene oxidn. to propylene oxide over Ag/TS-1 catalyst in gas phase)
- IT 1333-74-0, Hydrogen, uses 7727-37-9, Nitrogen, uses
(calcination atm. effect on propylene oxidn. to propylene oxide over Ag/TS-1 catalyst in gas phase)
- IT 13463-67-7, Titania, uses
(catalyst support effect on propylene oxidn. to propylene oxide over Ag/TS-1 catalyst in gas phase)
- IT 7631-86-9, Silica, reactions
(in prepn. of catalyst support, or as catalyst support; propylene oxidn. to propylene oxide over Ag/TS-1 catalyst in gas phase)
- IT 5593-70-4, Tetrabutyltitanate
(in prepn. of catalyst support; propylene oxidn. to propylene oxide over Ag/TS-1 catalyst in gas phase)
- IT 7761-88-8, Silver nitrate, reactions
(in prepn. of catalyst; propylene oxidn. to propylene oxide over Ag/TS-1 catalyst in gas phase)
- IT 7722-84-1, Hydrogen peroxide, reactions
7782-44-7, Oxygen, reactions

- (oxidant; propylene oxidn. to propylene oxide over Ag/TS-1 catalyst in gas phase)
- IT 67-64-1P, Acetone, preparation 107-02-8P, Acrolein, preparation 123-38-6P, Propanal, preparation **124-38-9P, Carbon dioxide**, preparation 1320-67-8P, Propylene glycol monomethyl ether
- (propylene oxidn. to propylene oxide over Ag/TS-1 catalyst in gas phase)
- IT 7440-22-4P, Silver, preparation
- (propylene oxidn. to propylene oxide over Ag/TS-1 catalyst in gas phase)
- IT 75-56-9P, Propylene oxide, preparation
- (propylene oxidn. to propylene oxide over Ag/TS-1 catalyst in gas phase)
- IT 115-07-1, Propylene, reactions
- (propylene oxidn. to propylene oxide over Ag/TS-1 catalyst in gas phase)
- IT 1941-30-6, Tetrapropylammonium bromide
- (template in prepn. of catalyst support; propylene oxidn. to propylene oxide over Ag/TS-1 catalyst in gas phase)

L66 ANSWER 5 OF 16 HCA COPYRIGHT 2006 ACS on STN

142:121134 Kinetic Study of a Direct Water Synthesis over Silica-Supported Gold Nanoparticles. Barton, David G.; Podkolzin, Simon G. (Core Research, The Dow Chemical Company, Midland, MI, 48674, USA). Journal of Physical Chemistry B, 109(6), 2262-2274 (English) 2005. CODEN: JPCBFK. ISSN: 1520-6106. Publisher: American Chemical Society.

AB The reaction mechanism of water formation from **H2** and **O2** was studied over a series of silica-supported gold nanoparticles. The metal particle size distributions were estd. with TEM and XRD measurements. Hydrogen and oxygen adsorption calorimetry was used to probe the nature and properties of surface species formed by these mols. DFT calcns. with Au5, Au13, and Au55 clusters and with Au(111) and Au(211) periodic slabs were performed to est. the thermodyn. stability and reactivity of surface species. Kinetic measurements were performed by varying the reactant partial pressures at 433 K and by varying the temp. from 383 to 483 K at 2.5 kPa of **O2** and 5 kPa of **H2**. The measured apparent power law kinetic parameters were similar for all catalysts in this study: hydrogen order of 0.7-0.8, oxygen order of 0.1-0.2, and activation energy of 37-41 kJ/mol. Catalysts with Si-MFI (Silicalite-1) and Ti-MFI (**TS-1** with 1 wt % Ti) exhibited similar activities. The activities of these catalysts with the MFI cryst. supports were 60-70 times higher than that of an analogous catalyst with an amorphous silica support. Water addn. in the inlet stream at 3 vol % did not affect the reaction rates. The

mechanism of water formation over gold is proposed to proceed through the **formation** of OOH and H₂O₂ intermediates. A rate expression derived based on this mechanism accurately describes the exptl. kinetic data. The higher activity of the MFI-supported catalysts is attributed to a higher concn. of gold particles comparable in size to Au₁₃, which can fit inside MFI pores. DFT results suggest that such intermediate-size gold particles are most reactive toward water formation. Smaller particles are proposed to be less reactive due to the instability of the OOH intermediate whereas larger particles are less reactive due to the instability of adsorbed oxygen.

IT 1333-74-0, Hydrogen, reactions 7782-44-7, Oxygen, reactions

(kinetics of direct water synthesis over silica-supported gold nanoparticles)

RN 1333-74-0 HCA

CN Hydrogen (8CI, 9CI) (CA INDEX NAME)

H-H

RN 7782-44-7 HCA

CN Oxygen (8CI, 9CI) (CA INDEX NAME)

O=O

CC 67-3 (Catalysis, Reaction Kinetics, and Inorganic Reaction Mechanisms)

Section cross-reference(s): 65, 66

IT Titanosilicate **zeolites**

(Ti-MFI; kinetics of direct water synthesis over silica-supported gold nanoparticles)

IT 1333-74-0, Hydrogen, reactions 7782-44-7, Oxygen, reactions

(kinetics of direct water synthesis over silica-supported gold nanoparticles)

L66 ANSWER 6 OF 16 HCA COPYRIGHT 2006 ACS on STN

141:146278 **Formation** of hydrogen **peroxide** from

H₂ and O₂ over a neutral gold trimer: a DFT study.

Wells, David H.; Delgass, W. Nicholas; Thomson, Kendall T. (School of Chemical Engineering, Purdue University, West Lafayette, IN, 47907, USA). Journal of Catalysis, 225(1), 69-77 (English) 2004. CODEN: JCTLA5. ISSN: 0021-9517. Publisher: Elsevier Science.

AB Our d.-functional theory study of the **formation** of hydrogen **peroxide** over a neutral Au₃ cluster details a reaction path with activation barriers less than 10 kcal/mol. The

reactions proceed on the edges and one side of the triangular Au₃ cluster which makes this mechanism viable for a cluster in contact with a support surface. The Au₃ cluster remains in a triangular geometry throughout the reaction but the electron population on the Au trimer during the catalytic cycle proper, as calcd. with the Natural Bond Orbital method, varies from a charge of +0.304 (cationic) (Au₃O₂H₂) to -0.138 (anionic) (Au₃H₂). Au₃ in the reaction initiation intermediate, Au₃O₂, is also cationic in character with a charge of +0.390. It is interesting to note that the interaction of Au₃ with a model oxidic support, TS-1, was essentially neutral in character, the Au₃ charge population being -0.044. **Formation** of hydrogen **peroxide** does not involve breaking the O-O bond, but does break the H-H bond in a step that is rate limiting under std. conditions. The highest energy barrier in the cycle is 8.6 kcal/mol for desorption of H₂O₂ from Au₃H₂. Adsorption of H₂O₂ on this site is unactivated. This route to **formation** of hydrogen **peroxide** combined with existing mechanisms for epoxidn. by H₂O₂ over TS-1 gives a fully plausible, energetically favorable, closed cycle for epoxidn. of propylene by H₂ and O₂ over Au/TS-1 catalysts. Thus, isolated mol. gold clusters can act as viable sites for this reaction.

IT 7722-84-1, Hydrogen **peroxide**, properties
(**formation** of hydrogen **peroxide** from
H₂ and O₂ over neutral gold trimer and DFT
study)
RN 7722-84-1 HCA
CN Hydrogen peroxide (H₂O₂) (9CI) (CA INDEX NAME)

HO-OH

IT 1333-74-0, Hydrogen, reactions 7782-44-7, Oxygen,
reactions
(**formation** of hydrogen **peroxide** from
H₂ and O₂ over neutral gold trimer and DFT
study)
RN 1333-74-0 HCA
CN Hydrogen (8CI, 9CI) (CA INDEX NAME)

H-H

RN 7782-44-7 HCA
CN Oxygen (8CI, 9CI) (CA INDEX NAME)

O=O

- CC 67-3 (Catalysis, Reaction Kinetics, and Inorganic Reaction Mechanisms)
Section cross-reference(s): 22, 23, 35, 45, 65, 66
- ST **formation** hydrogen **peroxide** neutral gold trimer
surface DFT catalyst; oxygen hydrogen reaction neutral gold trimer
surface DFT catalyst; epoxidn propylene mechanism gold TS1 zeolite catalyst
- IT Titanosilicate zeolites
(**TS-1**; **formation** of hydrogen **peroxide** from **H2** and **O2** over neutral gold trimer and DFT study)
- IT Molecular structure determination methods
(calcn.; **formation** of hydrogen **peroxide** from **H2** and **O2** over neutral gold trimer and DFT study)
- IT Adsorption
Density functional theory
Desorption
Electron density
Free energy
Internal energy
Partition function
Potential barrier
Surface reaction
Surface reaction kinetics
Transition state structure
Zero point energy
(**formation** of hydrogen **peroxide** from **H2** and **O2** over neutral gold trimer and DFT study)
- IT Epoxidation catalysts
(mechanism; **formation** of hydrogen **peroxide** from **H2** and **O2** over neutral gold trimer and DFT study)
- IT Clusters
(metal; **formation** of hydrogen **peroxide** from **H2** and **O2** over neutral gold trimer and DFT study)
- IT 115-07-1, Propylene, reactions
(epoxidn. of; **formation** of hydrogen **peroxide** from **H2** and **O2** over neutral gold trimer and DFT study)
- IT 7440-57-5, Gold, uses 514789-93-6, uses
(**formation** of hydrogen **peroxide** from

- H₂ and O₂ over neutral gold trimer and DFT study)
- IT 7722-84-1, Hydrogen **peroxide**, properties
(**formation** of hydrogen **peroxide** from
H₂ and O₂ over neutral gold trimer and DFT
study)
- IT 1333-74-0, Hydrogen, reactions 7782-44-7, Oxygen,
reactions
(**formation** of hydrogen **peroxide** from
H₂ and O₂ over neutral gold trimer and DFT
study)
- L66 ANSWER 7 OF 16 HCA COPYRIGHT 2006 ACS on STN
140:236121 **Production** of H₂O₂ in CO₂ and
its use in the direct synthesis of propylene oxide. Beckman, E. J.
(Chemical Engineering Dept., University of Pittsburgh, Pittsburgh,
PA, 15261, USA). Green Chemistry, 5(3), 332-336 (English) 2003.
CODEN: GRCHFJ. ISSN: 1463-9262. Publisher: Royal Society of
Chemistry.
- AB We have designed CO₂-sol. catalysts for **generating**
H₂O₂ from H₂ and O₂ in **carbon**
dioxide-water mixts. The use of supercrit. CO₂ as
solvent allows for use of reasonable concns. of H₂ and
O₂ and homogeneous catalysis eliminates diffusional
limitations to reaction. We have shown that H₂O₂
generated in situ from H₂ and O₂ in
CO₂ cleanly epoxidizes propylene to propylene oxide (PO).
PO is currently produced either via the chlorohydrin route, which
produces two pounds of waste per lb of PO, or via one of several
"peroxidn." processes, where a co-product must be produced with the
desired PO and hence waste vols. and energy requirements are much
higher than desired. Because those factors that render the current
AQ process for H₂O₂ less than green also contribute to its
relatively high cost, **generation** of H₂O₂ from
H₂ and O₂ in CO₂ not only permits green
synthesis of an important commodity, but also opens other
applications for use of this green oxidant.
- IT 7722-84-1P, Hydrogen **peroxide**,
preparation
(**prodn.** of H₂O₂ in CO₂ and its use
in direct synthesis of propylene oxide)
- RN 7722-84-1 HCA
CN Hydrogen peroxide (H₂O₂) (9CI) (CA INDEX NAME)

HO-OH

- IT 1333-74-0, Hydrogen, reactions 7782-44-7, Oxygen,

reactions

(starting material; **prodn.** of **H2O2** in
CO2 and its use in direct synthesis of propylene oxide)

RN 1333-74-0 HCA

CN Hydrogen (8CI, 9CI) (CA INDEX NAME)

H-H

RN 7782-44-7 HCA

CN Oxygen (8CI, 9CI) (CA INDEX NAME)

O=O

IT 124-38-9, **Carbon dioxide**, uses

(supercrit.; **prodn.** of **H2O2** in **CO2**
and its use in direct synthesis of propylene oxide)

RN 124-38-9 HCA

CN Carbon dioxide (8CI, 9CI) (CA INDEX NAME)

O=C=O

CC 35-2 (Chemistry of Synthetic High Polymers)
Section cross-reference(s): 27, 45, 49, 67

ST **hydrogen peroxide prodn** supercrit
carbon dioxide solvent; propylene epoxidn
hydrogen peroxide green generation

IT Titanium silicalite
(**TS-1**; in **prodn.** of **H2O2**
in **CO2**)

IT Catalysts
(for **prodn.** of **H2O2** from hydrogen and oxygen
in supercrit. **CO2**)

IT Green chemistry
(in **prodn.** of **H2O2** in **CO2** and its
use in direct synthesis of propylene oxide)

IT Epoxidation
(**prodn.** of **H2O2** in **CO2** and its use
in direct synthesis of propylene oxide)

IT Solvents
(supercrit.; **prodn.** of **H2O2** in **CO2**
and its use in direct synthesis of propylene oxide)

IT 13601-08-6
(catalyst precursor; in **prodn.** of **H2O2** in
CO2)

IT 75-56-9P, Propylene oxide, **preparation**

- (**prodn.** of **H2O2** in **CO2** and its use in direct synthesis of propylene oxide)
- IT 7722-84-1P, **Hydrogen peroxide, preparation**
 (**prodn.** of **H2O2** in **CO2** and its use in direct synthesis of propylene oxide)
- IT 115-07-1, **Propylene, reactions**
 (**prodn.** of **H2O2** in **CO2** and its use in direct synthesis of propylene oxide)
- IT 1333-74-0, **Hydrogen, reactions** 7782-44-7, **Oxygen, reactions**
 (starting material; **prodn.** of **H2O2** in **CO2** and its use in direct synthesis of propylene oxide)
- IT 124-38-9, **Carbon dioxide, uses**
 (supercrit.; **prodn.** of **H2O2** in **CO2** and its use in direct synthesis of propylene oxide)
- L66 ANSWER 8 OF 16 HCA COPYRIGHT 2006 ACS on STN
- 139:164424 Reactive oxygen species in epoxidation reactions over titanosilicate molecular sieves. Shetti, Vasudev N.; Manikandan, P.; Srinivas, D.; Ratnasamy, P. (National Chemical Laboratory, Pune, 411 008, India). Journal of Catalysis, 216(1-2), 461-467 (English) 2003. CODEN: JCTLA5. ISSN: 0021-9517. Publisher: Elsevier Science.
- AB In an attempt to rationalize the differences in the catalytic behavior of titanosilicate mol. sieves when using **H2O2** (**TS-1**, **TiMCM-41**) vs. **H2 + O2** (**Pd-TS-1**) as oxidant, the **Ti(IV)**-superoxo and hydroperoxo/peroxo species formed in situ during the oxidn. reactions were investigated by ESR (EPR) and diffuse reflectance UV-visible spectroscopies. Two types of superoxo species, A and B, were identified in **TS-1**; only the latter species was detected in **TiMCM-41**. EPR has provided evidence, for the first time, for the in situ generation of similar oxo species in reactions using **H2 + O2** instead of **H2O2**. The **Ti** sites adjacent to **Pd** ions (in **Pd-TS-1**) behave differently magnetically than the other **Ti** ions, generating a greater variety of superoxo species (**A'**, **A''**, **A**, **B'**, **B**, and **C**) and corresponding reaction products. **Pd** enhances the reducibility of **Ti** and promotes formation of these oxo species at lower temps. (.apprx. 323 K). The epoxide selectivity in the oxidn. of allyl alc. over **Pd-TS-1** is higher when using (**H2 + O2**) than when using **H2O2**. In all cases, type A species predominantly catalyze epoxidns. while type B favor the hydroxylations. The selectivity for epoxidn. (vis-a-vis allylic oxidn.) over these catalysts can be enhanced by controlling the type of **Ti**-oxo species formed in situ during the oxidn. process by a

suitable combination of catalyst, oxidant, solvent, and temp.

IT 7440-05-3, Palladium, uses
(reactive oxygen species in epoxidn. reactions over
titanosilicate mol. sieves)

RN 7440-05-3 HCA

CN Palladium (8CI, 9CI) (CA INDEX NAME)

Pd

IT 7722-84-1, **Hydrogen peroxide**, reactions
(reactive oxygen species in epoxidn. reactions over
titanosilicate mol. sieves)

RN 7722-84-1 HCA

CN Hydrogen peroxide (H2O2) (9CI) (CA INDEX NAME)

HO-OH

CC 22-7 (Physical Organic Chemistry)

Section cross-reference(s): 67

ST epoxidn allyl alc titanosilicate catalyst reactive species
ESR

IT 7440-05-3, Palladium, uses
(reactive oxygen species in epoxidn. reactions over
titanosilicate mol. sieves)

IT 107-18-6, Allyl **alcohol**, reactions
(reactive oxygen species in epoxidn. reactions over
titanosilicate mol. sieves)

IT 7722-84-1, **Hydrogen peroxide**, reactions
(reactive oxygen species in epoxidn. reactions over
titanosilicate mol. sieves)

L66 ANSWER 9 OF 16 HCA COPYRIGHT 2006 ACS on STN

137:232942 Study on process integration of the production of propylene
oxide and **hydrogen peroxide**. Wang, Chunyan;
Wang, Baoguo; Meng, Xiangkun; Mi, Zhentao (School of Chemical
Engineering and Technology, Tianjin University, Tianjin, 300072,
Peop. Rep. China). Catalysis Today, 74(1-2), 15-21 (English) 2002.
CODEN: CATTEA. ISSN: 0920-5861. Publisher: Elsevier Science B.V..
AB Titanium silicalite (TS-1) is an effective
catalyst for selective oxidn. of hydrocarbons and their derivs. with
hydrogen peroxide under mild conditions. The
industrialization of these processes is at present penalized by the
high cost of **hydrogen peroxide**. The process
integration of the prodn. of propylene oxide (PO) with the
prodn. of hydrogen peroxide (
H2O2) by the anthraquinone route is presented in this paper.

Two integrated processes are discussed: in the first process, the solvent for the epoxidn. step is recycled to ext. **H2O2** from the anthraquinone working soln.; while in the second process, two oxidn. processes, the epoxidn. of propylene and the oxidn. of anthrahydroquinone, are carried out in one circulating reactor. The influences of various reagents on the performance of **TS-1** and the compatibility of the two oxidn. processes were investigated. The results show that it is better to integrate the prodn. of PO with the **prodn.** of **H2O2** when **TS-1** is used as catalyst.

IT 7782-44-7, Oxygen, reactions
(in integrated prodn. of propylene oxide and **hydrogen peroxide**)
RN 7782-44-7 HCA
CN Oxygen (8CI, 9CI) (CA INDEX NAME)

O=O

IT 7722-84-1P, **Hydrogen peroxide, preparation**
(integrated **prodn.** of propylene oxide and **hydrogen peroxide**)
RN 7722-84-1 HCA
CN Hydrogen peroxide (H2O2) (9CI) (CA INDEX NAME)

HO-OH

IT 67-56-1, **Methanol**, uses
(solvent; in integrated prodn. of propylene oxide and **hydrogen peroxide**)
RN 67-56-1 HCA
CN Methanol (8CI, 9CI) (CA INDEX NAME)

H₃C-OH

CC 35-2 (Chemistry of Synthetic High Polymers)
Section cross-reference(s): 27, 45, 49, 67
ST propylene epoxidn **hydrogen peroxide**
prodn process integration; titanium silicalite
catalyst propylene oxide **hydrogen peroxide**
coprodn
IT Titanium silicalite
(**TS-1**; catalyst in integrated prodn. of
propylene oxide and **hydrogen peroxide**)
IT Epoxidation catalysts

- (in integrated prodn. of propylene oxide and **hydrogen peroxide**)
- IT 84-65-1, Anthraquinone 4981-66-2, Anthrahydroquinone
(in integrated prodn. of propylene oxide and **hydrogen peroxide**)
- IT 115-07-1, Propylene, reactions 7782-44-7, Oxygen, reactions
(in integrated prodn. of propylene oxide and **hydrogen peroxide**)
- IT 75-56-9P, Propylene oxide, preparation 7722-84-1P, **Hydrogen peroxide, preparation**
(integrated prodn. of propylene oxide and **hydrogen peroxide**)
- IT 67-56-1, **Methanol**, uses 7732-18-5, Water, uses
(solvent; in integrated prodn. of propylene oxide and **hydrogen peroxide**)
- L66 ANSWER 10 OF 16 HCA COPYRIGHT 2006 ACS on STN
- 134:33383 Redox and catalytic chemistry of Ti in titanosilicate molecular sieves: an EPR investigation. Bal, R.; Chaudhari, K.; Srinivas, D.; Sivasanker, S.; Ratnasamy, P. (National Chemical Laboratory, Pune, 411008, India). Journal of Molecular Catalysis A: Chemical, 162(1-2), 199-207 (English) 2000. CODEN: JMCCF2. ISSN: 1381-1169. Publisher: Elsevier Science B.V..
- AB An EPR study of Ti³⁺ in titanosilicate mol. sieves, **TS-1**, TiMCM-41, ETS-10 and ETS-4 is reported. Ti⁴⁺ is reduced to Ti³⁺ by dry hydrogen above 673 K. Ti ions in **TS-1** and TiMCM-41 are located in tetragonally elongated Td and those of ETS-10 and ETS-4 in a tetragonally compressed Oh geometric positions. Redn. at 873 K revealed the presence of two non-equiv. Ti³⁺ sites in **TS-1** and TiMCM-41. Ti⁴⁺ ions in a tetrahedral geometry are more difficult to reduce than in an octahedral symmetry. The effects of cation exchange and **Pt** impregnation, on the geometry and reducibility of titanium in ETS-10, are also examd. Interaction of a tetrahedrally coordinated Ti³⁺ with **O2** or **H2O2** results in a diamagnetic titanium(IV) hydroperoxo species. Under the same conditions, an octahedrally coordinated Ti³⁺ forms a paramagnetic titanium(IV) superoxo species. The higher catalytic activity of **TS-1** and TiMCM-41 in selective oxidn. reactions is probably a consequence of the formation of the hydroperoxy species on their surface during the catalytic reaction. The presence of **Pt** in the vicinity of Ti enables the use of **H2** and **O2** (instead of **H2O2**) to **generate** the active hydroperoxy site. The absence of formation of titanium hydroperoxy species in ETS-4 and ETS-10 is the cause of their inactivity in selective oxidn. reactions.
- CC 67-1 (Catalysis, Reaction Kinetics, and Inorganic Reaction

Mechanisms)

Section cross-reference(s): 77

- ST titanium redox chem titanasilicate zeolite mol sieve catalyst ESR;
TS1 mol sieve catalyst titanium redox chem ESR; TiMCM41 mol
sieve catalyst titanium redox chem ESR; ETS10 mol sieve catalyst
titanium redox chem ESR; ETS4 mol sieve catalyst titanium redox chem
ESR
- IT Titanasilicate zeolites
(**TS-1**; redox and catalytic chem. of Ti in
titanasilicate mol. sieves and EPR investigation)

L66 ANSWER 11 OF 16 HCA COPYRIGHT 2006 ACS on STN

132:37253 Direct hydroxylation of aromatics by hydrogen and oxygen.

Lee, Kew-Ho; Jegal, Jonggeon (Korea Research Institute of Chemical
Technology, S. Korea). PCT Int. Appl. WO 9964129 A2 19991216, 17
pp. DESIGNATED STATES: W: JP, US; RW: AT, BE, CH, CY, DE, DK, ES,
FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE. (English). CODEN:
PIXXD2. APPLICATION: WO 1999-KR283 19990609. PRIORITY: KR
1998-21396 19980610.

- AB The present invention relates to a process for prepg. hydroxylated
aroms. by using hydrogen and oxygen and more particularly, to a
process for prepg. hydroxylated aroms. by using hydrogen and oxygen
with a two-component heterogeneous catalyst. One component consists
of porous catalyst contg. one of Group VIII B transition metals such
as **Pd**, **Pt**, **Au**, and **Cu**, and hydrogen-transfer
org. compds. such as anthraquinone. The other component consists of
a catalyst contg. a transition metal selected from **Ti**, **V**, and **Sn**
with tetrahedral coordination geometry. The main advantages of this
new catalytic system are to (1) overcome the drawbacks of liq. phase
oxidn. using conventional homogeneous catalysts, (2) avoid use of
expensive **hydrogen peroxide** as an oxidant, and
(3) improve the selectivity of the reaction. In an example, **PhOH** is
produced from 15 mL benzene using 0.25 g **Y zeolite** contg.
2-ethylanthraquinone and **Pd** and 0.25 g **Y zeolite**
contg. **Ti**.

- IT **1333-74-0**, Hydrogen, reactions **7782-44-7**, Oxygen,
reactions
(direct hydroxylation of aroms. by hydrogen and oxygen using
zeolite catalyst)

RN 1333-74-0 HCA

CN Hydrogen (8CI, 9CI) (CA INDEX NAME)

H-H

RN 7782-44-7 HCA

CN Oxygen (8CI, 9CI) (CA INDEX NAME)

O=O

IT 7440-05-3, Palladium, uses 7440-06-4, Platinum,
uses
(direct hydroxylation of aro. by hydrogen and oxygen using
zeolite catalyst contg.)

RN 7440-05-3 HCA

CN Palladium (8CI, 9CI) (CA INDEX NAME)

Pd

RN 7440-06-4 HCA

CN Platinum (8CI, 9CI) (CA INDEX NAME)

Pt

IC ICM B01D

CC 45-4 (Industrial Organic Chemicals, Leather, Fats, and Waxes)
Section cross-reference(s): 67

ST benzene direct hydroxylation oxygen hydrogen use; phenol prodn
zeolite hydroxylation catalyst; **palladium** titanium
anthraquinone **catalyst** hydroxylation benzene

IT 1333-74-0, Hydrogen, reactions 7782-44-7, Oxygen,
reactions
(direct hydroxylation of aro. by hydrogen and oxygen using
zeolite catalyst)

IT 84-51-5, 2-Ethylantraquinone 84-65-1D, Anthraquinone, alkyl
derivs. 117-78-2, 2-Anthraquinonecarboxylic acid 853-35-0,
Disodium 1,5-anthraquinonedisulfonate 7440-05-3,
Palladium, uses 7440-06-4, Platinum, uses 7440-31-5,
Tin, uses 7440-32-6, Titanium, uses 7440-50-8, Copper, uses
7440-57-5, Gold, uses 7440-62-2, Vanadium, uses 7504-51-0,
2-Butylantraquinone 13936-21-5, 2-Amylantraquinone
(direct hydroxylation of aro. by hydrogen and oxygen using
zeolite catalyst contg.)

L66 ANSWER 12 OF 16 HCA COPYRIGHT 2006 ACS on STN

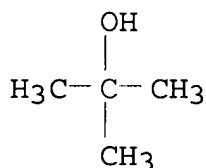
131:300745 Vapor-Phase Selective Oxidation of Aliphatic Hydrocarbons
over Gold Deposited on Mesoporous Titanium Silicates in the
Co-Presence of Oxygen and Hydrogen. Kalvachev, Yuri Angelov;
Hayashi, Toshio; Tsubota, Susumu; Haruta, Masatake (Osaka National
Research Institute, AIST, Ikeda, 563-8577, Japan). Journal of
Catalysis, 186(1), 228-233 (English) 1999. CODEN: JCTLA5. ISSN:
0021-9517. Publisher: Academic Press.

AB The catalytic activity of Au deposited on Ti-MCM-41 and on TiO₂

dispersed on silica was evaluated in epoxidn. of propylene and in selective oxidn. of propane to acetone and of isobutane to t-butanol with a H₂-O₂ mixt. under flow.

The oxidn. of propylene showed a relatively long induction period, about 1.5 h at 373 K and becomes longer at 323 K; H consumption is about double that over Au/TiO₂/O₂. The proposed reaction mechanism involves coverage of the surface of Au particles by the hydrocarbon; at the Au surface, H₂O₂ forms from H and O and migrates to free Ti sites where it is transformed to the hydroperoxo species. The hydrocarbon adsorbed on the surface of the catalyst then reacts with the hydroperoxo species to yield **oxygenates**. (c) 1999 Academic Press.

- IT 75-65-0P, tert-Butanol, preparation
(vapor-phase selective oxidn. of aliph. hydrocarbons over gold deposited on mesoporous titanium silicates in Co-presence of oxygen and hydrogen)
- RN 75-65-0 HCA
- CN 2-Propanol, 2-methyl- (9CI) (CA INDEX NAME)



- CC 45-4 (Industrial Organic Chemicals, Leather, Fats, and Waxes)
Section cross-reference(s): 67
- ST gold **titanium** MCM41 **zeolite** catalyst selective oxidn hydrocarbon; propylene epoxidn gold **titanium zeolite** catalyst; propane oxidn acetone manuf gold **titanium zeolite** catalyst; isobutane oxidn catalyst **formation hydrogen peroxide**
- IT **Zeolite** MCM-41
(**titanium**-exchanged, support; vapor-phase selective oxidn. of aliph. hydrocarbons over gold deposited on mesoporous titanium silicates in Co-presence of oxygen and hydrogen)
- IT 67-64-1P, Acetone, preparation 75-56-9P, Propylene oxide, preparation 75-65-0P, tert-Butanol, preparation
(vapor-phase selective oxidn. of aliph. hydrocarbons over gold deposited on mesoporous titanium silicates in Co-presence of oxygen and hydrogen)

L66 ANSWER 13 OF 16 HCA COPYRIGHT 2006 ACS on STN
126:74861 Oxidation process and catalysts for the preparation of amine oxides from amines. Mueller, Ulrich; Massonne, Klemens; Eller, Karsten; Schulz, Michael (BASF A.-G., Germany). Eur. Pat. Appl. EP 745587 A1 19961204, 13 pp. DESIGNATED STATES: R: BE, DE, FR, GB,

IT, NL. (German). CODEN: EPXXDW. APPLICATION: EP 1996-108220
19960523. PRIORITY: DE 1995-19520270 19950602.

AB Amine oxides O:N(R1)(R2)R3 [R1-R3 = (un)substituted alkyl,
cycloalkyl, (un)substituted aryl, etc.; R1R2 may form a O- or
S-contg. chain] (e.g., N-methylmorpholine oxide) are prepd. without
the use of H₂O₂ by oxidn. of amines R1N(R2)R3 (e.g.,
N-methylmorpholine) in the presence of a H₂/O₂
gas mixt. and an oxidn. catalyst comprising a Group VIIIB metal
(e.g., Pd) on a **zeolitic titanium**
silicate or vanadium silicate support.

IT **7440-05-3**, Palladium, uses **7440-06-4**, Platinum,
uses
(oxidn. process and catalysts for the prepn. of amine oxides from
amines)

RN 7440-05-3 HCA
CN Palladium (8CI, 9CI) (CA INDEX NAME)

Pd

RN 7440-06-4 HCA
CN Platinum (8CI, 9CI) (CA INDEX NAME)

Pt

IC ICM C07C291-04
CC 28-13 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 21, 23, 25, 45, 67

IT Oxidation catalysts
(Group VIIIB metal on a **zeolitic titanium**
silicate or vanadium silicate for the prepn. of amine oxides from
amines)

IT Group VIII elements
(catalytic Group VIIIB metals on a **zeolitic**
titanium silicate or vanadium silicate for the prepn. of
amine oxides from amines)

IT 7439-88-5, Iridium, uses 7440-04-2, Osmium, uses **7440-05-3**
, Palladium, uses **7440-06-4**, Platinum, uses 7440-15-5,
Rhenium, uses 7440-16-6, Rhodium, uses 7440-18-8, Ruthenium,
uses 7440-22-4, Silver, uses 7440-57-5, Gold, uses 12653-89-3,
Vanadium silicate 42613-21-8, Titanium silicate
(oxidn. process and catalysts for the prepn. of amine oxides from
amines)

L66 ANSWER 14 OF 16 HCA COPYRIGHT 2006 ACS on STN
125:304529 Process for manufacturing **zeolites Ti**
-.beta., and the zeolites obtained and their use. Corma, Avelino;

Camblor, Miguel Angel; Perez Pariente, Joaquin; Valencia, Susana; Costantini, Michel; Gilbert, Laurent (Rhone-Poulenc Chimie SA, Fr.).

Fr. Demande FR 2730722 A1 19960823, 22 pp. (French). CODEN: FRXXBL. APPLICATION: FR 1995-1823 19950217.

AB The process comprises adding zeolite .beta.-type alumino-, ferro-, gallo- and/or borosilicates as crystn. agents to a reaction mixt. comprising a source of Si, a source of Ti, a templating agent, and a mobilizing agent, and hydrothermally crystg. and recovering the zeolite from the mixt. The calcined, anhyd. zeolites have compn. $\text{HXO}_2 \cdot \text{bTiO}_2 \cdot \text{aSiO}_2$ ($\text{a} = >100$ but <5000 ; $\text{b/a} >0$ but ≤ 0.05 ; X = trivalent element, e.g., Al, Fe, Ga, B; H may be replaced, at least partially, by other cations). The zeolites are used as catalysts for selectively oxidizing org. compds. with H_2O_2 or org. peroxides or hydroperoxides, esp. the hydroxylation of phenols and phenol ethers with H_2O_2 .

IT 7722-84-1, Hydrogen peroxide, processes
(zeolites Ti-.beta. manuf. for use as catalysts for oxidizing org. compds. and for hydroxylating phenols and phenol ethers with)

RN 7722-84-1 HCA

CN Hydrogen peroxide (H_2O_2) (9CI) (CA INDEX NAME)

HO-OH

IC ICM C01B039-06

ICS B01J029-89; C07B041-02; C07C037-60; C07C039-08

CC 49-4 (Industrial Inorganic Chemicals)

ST zeolite titanasilicate beta titanium substituted; catalyst oxidn hydroxylation zeolite Ti beta; phenol hydroxylation catalyst hydrogen peroxide; ether phenol hydroxylation catalyst; crystn agent zeolite catalyst; aluminosilicate crystn agent zeolite; ferrosilicate crystn agent zeolite; gallosilicate crystn agent zeolite; borosilicate crystn agent zeolite

IT Hydroxylation catalysts

Oxidation catalysts

(zeolites Ti-.beta. manuf. for use as catalysts for oxidizing org. compds. and for hydroxylating phenols and phenol ethers with)

IT Phenols, processes

Titanium halides

(zeolites Ti-.beta. manuf. for use as catalysts for oxidizing org. compds. and for hydroxylating phenols and phenol ethers with)

IT Zeolites, uses

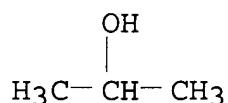
(.beta.-type, crystn. agents; zeolites Ti

- .beta. manuf. for use as catalysts for oxidizing org. compds. and for hydroxylating phenols and phenol ethers with)
- IT Ethers, processes
(Ph, **zeolites Ti-.beta.** manuf. for use as catalysts for oxidizing org. compds. and for hydroxylating phenols and phenol ethers with)
- IT Crystallization
(agents, **zeolites Ti-.beta.** manuf. for use as catalysts for oxidizing org. compds. and for hydroxylating phenols and phenol ethers with)
- IT **Zeolites**, preparation
(beta, **titanium**-substituted, **zeolites Ti-.beta.** manuf. for use as catalysts for oxidizing org. compds. and for hydroxylating phenols and phenol ethers with)
- IT Zeolites, uses
(borosilicate, .beta.-type, crystn. agents; **zeolites Ti-.beta.** manuf. for use as catalysts for oxidizing org. compds. and for hydroxylating phenols and phenol ethers with)
- IT Zeolites, uses
(ferrisilicate, .beta.-type, crystn. agents; **zeolites Ti-.beta.** manuf. for use as catalysts for oxidizing org. compds. and for hydroxylating phenols and phenol ethers with)
- IT Zeolites, uses
(gallosilicate, .beta.-type, crystn. agents; **zeolites Ti-.beta.** manuf. for use as catalysts for oxidizing org. compds. and for hydroxylating phenols and phenol ethers with)
- IT Crystallization
(hydrothermal, **zeolites Ti-.beta.** manuf. for use as catalysts for oxidizing org. compds. and for hydroxylating phenols and phenol ethers with)
- IT Bases, uses
(org., templating agent; **zeolites Ti-.beta.** manuf. for use as catalysts for oxidizing org. compds. and for hydroxylating phenols and phenol ethers with)
- IT Hydroperoxides
Peroxides, processes
(org., **zeolites Ti-.beta.** manuf. for use as catalysts for oxidizing org. compds. and for hydroxylating phenols and phenol ethers with)
- IT **Alcohols**, processes
(**titanium** salts, **zeolites Ti-.beta.** manuf. for use as catalysts for oxidizing org. compds. and for hydroxylating phenols and phenol ethers with)
- IT 7631-86-9, Silica, processes
(colloidal; **zeolites Ti-.beta.** manuf. for use as catalysts for oxidizing org. compds. and for hydroxylating phenols and phenol ethers with)
- IT 60676-86-0, Vitreous silica

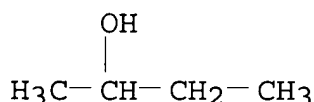
- (fume; **zeolites Ti-.beta.** manuf. for use as catalysts for oxidizing org. compds. and for hydroxylating phenols and phenol ethers with)
- IT 77-98-5, Tetraethylammonium hydroxide 6249-58-7,
Dibenzyltrimethylammonium hydroxide
(templating agent; **zeolites Ti-.beta.** manuf. for use as catalysts for oxidizing org. compds. and for hydroxylating phenols and phenol ethers with)
- IT 78-10-4, Tetraethyl orthosilicate 90-05-1, 2-Methoxyphenol
95-48-7, **o**-Cresol, **processes** 98-54-4,
4-tert.-Butylphenol 100-66-3, Anisole, **processes** 106-44-5,
p-Cresol, **processes** 108-39-4, **processes** 108-95-2, Phenol,
processes 3087-36-3, **Titanium** tetraethoxide 5593-70-4,
Titanium tetrabutoxide 7446-70-0, Aluminum chloride,
processes 7550-45-0, **Titanium** tetrachloride, **processes**
7722-84-1, Hydrogen peroxide,
processes 13473-90-0, Aluminum nitrate
(**zeolites Ti-.beta.** manuf. for use as catalysts for oxidizing org. compds. and for hydroxylating phenols and phenol ethers with)
- L66 ANSWER 15 OF 16 HCA COPYRIGHT 2006 ACS on STN
- 122:315336 Integrated process for epoxide production. Zajacek, John G.;
Jubin, John C., Jr.; Crocco, Guy L. (Arco Chemical Technology, L.P.,
USA). U.S. US 5384418 A 19950124, 9 pp. Cont.-in-part of U.S. Ser.
No. 186,716, abandoned. (English). CODEN: USXXAM. APPLICATION: US
1994-241215 19940510. PRIORITY: US 1994-186716 19940125.
- AB Epoxides are produced by an integrated **process** involving
mol. **oxygen** oxidn. of an aliph. secondary **alc.**,
sepn. of the ketone co-product, epoxidn. of an ethylenically unsatd.
substrate by the substantially ketone-free oxidn. product in the
presence of a titanium silicalite catalyst, and regeneration of the
secondary **alc.** by **hydrogenation** of the ketone
co-product.
- IT **7722-84-1P, Hydrogen peroxide,**
preparation
(integrated process for epoxide prodn.)
- RN 7722-84-1 HCA
- CN Hydrogen peroxide (H2O2) (9CI) (CA INDEX NAME)

HO-OH

- IT 67-63-0, Isopropanol, reactions 78-92-2,
sec-Butanol
(integrated process for epoxide prodn.)
- RN 67-63-0 HCA
- CN 2-Propanol (9CI) (CA INDEX NAME)



RN 78-92-2 HCA
CN 2-Butanol (9CI) (CA INDEX NAME)



IC ICM C07D301-12
ICS C07D303-04
INCL 549531000
CC 35-2 (Chemistry of Synthetic High Polymers)
ST epoxide prepn secondary alc oxidn; titanium silicalite catalyst epoxide prepn
IT **Alcohols**, reactions
(aliph., secondary, integrated process for epoxide prodn.)
IT **Zeolites**, uses
(titanium silicalite, integrated process for epoxide prodn.)
IT **7722-84-1P, Hydrogen peroxide**,
preparation
(integrated process for epoxide prodn.)
IT **67-63-0, Isopropanol**, reactions **78-92-2**,
sec-Butanol
(integrated process for epoxide prodn.)

L66 ANSWER 16 OF 16 HCA COPYRIGHT 2006 ACS on STN
121:204656 Oxidation of hydrocarbons by oxygen and hydrogen over
Pd-containing titanium silicalites. Tatsumi, T.; Yuasa, K.;
Asano, K. (Fac. Eng., Univ. Tokyo, Tokyo, 113, Japan). Act.
Dioxygen Homogeneous Catal. Oxid., [Proc. Int. Symp.], 5th, 485.
Editor(s): Barton, Derek H. R.; Martell, Arthur Earl; Sawyer, Donald
T. Plenum: New York, N. Y. (English) 1993. CODEN: 60ENAZ.

AB A symposium in which the effects of solvent and catalysts on the
hydroxylation of benzene to phenol or of hexane to 2- and 3-hexanol
in 2-phase systems were discussed. Shape selectivity was found in
the oxidn. of alkanes and alkenes by **H2O2** over titanium
silicalite. The rates of linear alkene and alkane oxidns. were
faster than those of cycloalkenes and cycloalkanes. The catalytic
activity of the zeolitic catalysts was discussed.

IT **1333-74-0, Dihydrogen**, reactions **7722-84-1**,
Hydrogen peroxide, reactions **7782-44-7**,

Dioxygen, reactions

(oxidn. of hydrocarbons by oxygen and hydrogen over **Pd**
-contg. titanium silicalites in 2-phase systems)

RN 1333-74-0 HCA

CN Hydrogen (8CI, 9CI) (CA INDEX NAME)

H-H

RN 7722-84-1 HCA

CN Hydrogen peroxide (H₂O₂) (9CI) (CA INDEX NAME)

HO-OH

RN 7782-44-7 HCA

CN Oxygen (8CI, 9CI) (CA INDEX NAME)

O=O

IT 67-56-1, **Methanol**, uses 75-65-0, **tert-Butanol**, uses

(solvent; oxidn. of hydrocarbons by oxygen and hydrogen over
Pd-contg. titanium silicalites in 2-phase systems)

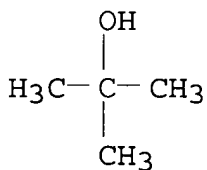
RN 67-56-1 HCA

CN Methanol (8CI, 9CI) (CA INDEX NAME)

H₃C-OH

RN 75-65-0 HCA

CN 2-Propanol, 2-methyl- (9CI) (CA INDEX NAME)

IT 7440-05-3, **Palladium**, uses

(zeolitic and carbon supported; oxidn. of hydrocarbons by oxygen
and hydrogen over **Pd**-contg. titanium silicalites in
2-phase systems)

RN 7440-05-3 HCA

CN Palladium (8CI, 9CI) (CA INDEX NAME)

- Pd
- CC 22-7 (Physical Organic Chemistry)
- ST oxidn hydrocarbon oxygen hydrogen zeolite symposium;
palladium titanium silicalite **catalyst** oxidn
symposium
- IT Kinetics of oxidation
Oxidation
Oxidation, aut-
Oxidation catalysts
(Oxidn. of hydrocarbons by oxygen and hydrogen over **Pd**
-contg. titanium silicalites)
- IT Solvent effect
(on oxidn. of hydrocarbons by oxygen and hydrogen over **Pd**
-contg. titanium silicalites in 2-phase systems)
- IT Hydroxylation
Hydroxylation catalysts
Kinetics of hydroxylation
(oxidn. of hydrocarbons by oxygen and hydrogen over **Pd**
-contg. titanium silicalites)
- IT Alkanes, reactions
Alkenes, reactions
Cycloalkanes
Cycloalkenes
Hydrocarbons, reactions
(oxidn. of hydrocarbons by oxygen and hydrogen over **Pd**
-contg. titanium silicalites)
- IT **Zeolites**, uses
(**palladium titanium** silicalite; oxidn. of hydrocarbons
by oxygen and hydrogen over **Pd**-contg. titanium
silicalites)
- IT Kinetics of oxidation
Oxidation catalysts
(aut-, Oxidn. of hydrocarbons by oxygen and hydrogen over
Pd-contg. titanium silicalites)
- IT **Zeolites**, uses
(**titanium** silicalite, oxidn. of hydrocarbons by oxygen
and hydrogen over **Pd**-contg. titanium silicalites)
- IT 71-43-2, Benzene, reactions 110-54-3, Hexane, reactions
(hydroxylation; oxidn. of hydrocarbons by oxygen and hydrogen
over **Pd**-contg. titanium silicalites in 2-phase systems)
- IT 1333-74-0, Dihydrogen, reactions 7722-84-1,
Hydrogen peroxide, reactions 7782-44-7,
Dioxygen, reactions
(oxidn. of hydrocarbons by oxygen and hydrogen over **Pd**
-contg. titanium silicalites in 2-phase systems)
- IT 108-95-2P, Phenol, preparation 623-37-0P, 3-Hexanol 626-93-7P,

2-Hexanol

(oxidn. of hydrocarbons by oxygen and hydrogen over **Pd**
-contg. titanium silicalites in 2-phase systems)

IT 67-56-1, **Methanol**, uses 75-65-0, tert-
Butanol, uses

(solvent; oxidn. of hydrocarbons by oxygen and hydrogen over
Pd-contg. titanium silicalites in 2-phase systems)

IT 7440-05-3, **Palladium**, uses

(zeolitic and carbon supported; oxidn. of hydrocarbons by oxygen
and hydrogen over **Pd**-contg. titanium silicalites in
2-phase systems)

IT 7440-32-6, **Titanium**, uses

(**zeolitic**; oxidn. of hydrocarbons by oxygen and
hydrogen over **Pd**-contg. titanium silicalites in 2-phase
systems)

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L67 ANSWER 1 OF 20 HCA COPYRIGHT 2006 ACS on STN

143:230359 Epoxidation catalyst regeneration process. Grey, Roger A.;
Kaminsky, Mark P. (USA). U.S. Pat. Appl. Publ. US 2005187095 A1
20050825, 8 pp. (English). CODEN: USXXCO. APPLICATION: US
2004-785455 20040224.

AB Used noble metal-contg. **Ti zeolite** catalysts,
that were employed in the liq.-phase epoxidn. of olefins with H and
O in the presence of a buffer, are regenerated by heating the used
catalyst at .gtoreq.250.degree. in the presence of a O
-contg. **gas stream**, followed by redn. at
.gtoreq.20.degree. in the presence of a H-contg.
gas stream to form a reactivated catalyst.

IT 1333-74-0, Hydrogen, reactions 7782-44-7, Oxygen,
reactions

(for spent noble metal-contg. epoxidn. catalyst regeneration)

RN 1333-74-0 HCA

CN Hydrogen (8CI, 9CI) (CA INDEX NAME)

H-H

RN 7782-44-7 HCA

CN Oxygen (8CI, 9CI) (CA INDEX NAME)

O=O

IT 7440-06-4, **Platinum**, uses

(spent noble metal-contg. epoxidn. catalyst regeneration)

RN 7440-06-4 HCA
CN Platinum (8CI, 9CI) (CA INDEX NAME)

Pt

IC ICM B01J038-18
INCL 502050000
CC 35-2 (Chemistry of Synthetic High Polymers)
Section cross-reference(s): 45, 67
IT Titanium silicalite
(TS-1; spent noble metal-contg. epoxidn.
catalyst regeneration)
IT 1333-74-0, Hydrogen, reactions 7782-44-7, Oxygen,
reactions
(for spent noble metal-contg. epoxidn. catalyst regeneration)
IT 7440-06-4, Platinum, uses 7440-57-5, Gold, uses
(spent noble metal-contg. epoxidn. catalyst regeneration)

L67 ANSWER 2 OF 20 HCA COPYRIGHT 2006 ACS on STN
140:289174 Cu²⁺-Exchanged Zeolites as Catalysts for Phenol Hydroxylation
with **Hydrogen Peroxide**. Wang, Jun; Park,
Jung-Nam; Jeong, Han-Cheol; Choi, Kwang-Sik; Wei, Xian-Yong; Hong,
Suk-In; Lee, Chul Wee (Advanced Chemical Technology Division, Korea
Research Institute of Chemical Technology, Daejeon, 305-600, S.
Korea). Energy & Fuels, 18(2), 470-476 (English) 2004. CODEN:
ENFUEM. ISSN: 0887-0624. OTHER SOURCES: CASREACT 140:289174.
Publisher: American Chemical Society.

AB The Cu²⁺-exchanged NaY, HY, USHY, H.beta., and HZSM-5 zeolites were
prepd. and evaluated in phenol hydroxylation with **hydrogen
peroxide** using an atm. batch reactor. CuNaY, CuHY, and
CuH.beta. catalysts were found to be more active than TS-
1 or a simple homogeneous copper nitrate catalyst under
similar reaction conditions. Both zeolite type and copper content
in the zeolite catalyst were revealed to exert crit. impact upon the
catalytic activity in phenol hydroxylation. Reaction time, reaction
temp., and the molar ratio of phenol to **hydrogen
peroxide** also remarkably influenced the reaction results.
The addn. of a small amt. of hydrochloric acid to the reaction
systems significantly enhanced the phenol conversion, hydroxylation
selectivity, and reaction rate. The used catalysts can be
regenerated completely by calcination at 450 .degree.C for 4 h in
air. On the basis of ESR spectroscopy, the relationship
between catalytic activity and copper loading is explained and the
hydroxyl radical is suggested as the reaction intermediate.

IT 7722-84-1, **Hydrogen peroxide**, reactions
(Cu²⁺-exchanged zeolites as catalysts for phenol hydroxylation
with **hydrogen peroxide**)

RN 7722-84-1 HCA
 CN Hydrogen peroxide (H2O2) (9CI) (CA INDEX NAME)

HO-OH

- CC 45-4 (Industrial Organic Chemicals, Leather, Fats, and Waxes)
 Section cross-reference(s): 67
- ST copper exchanged zeolite phenol **hydrogenation**
hydrogen peroxide hydrochloric acid; regeneration
 copper zeolite catechol hydroquinone benzoquinone prodn
- IT Zeolite CuZSM-5
 Zeolite HZSM-5
 (CuHZSM-5; Cu²⁺-exchanged zeolites as catalysts for phenol
 hydroxylation with **hydrogen peroxide**)
- IT Zeolite NaY
 (CuNaY; Cu²⁺-exchanged zeolites as catalysts for phenol
 hydroxylation with **hydrogen peroxide**)
- IT Hydroxylation catalysts
 (Cu²⁺-exchanged zeolites as catalysts for phenol hydroxylation
 with **hydrogen peroxide**)
- IT H-Beta zeolites
 (Cu²⁺-exchanged zeolites as catalysts for phenol hydroxylation
 with **hydrogen peroxide**)
- IT Ultrastable Y zeolites
 (HY; Cu²⁺-exchanged zeolites as catalysts for phenol
 hydroxylation with **hydrogen peroxide**)
- IT Zeolite HY
 (ultrastable; Cu²⁺-exchanged zeolites as catalysts for phenol
 hydroxylation with **hydrogen peroxide**)
- IT 7647-01-0, Hydrochloric acid, uses
 (Cu²⁺-exchanged zeolites as catalysts for phenol hydroxylation
 with **hydrogen peroxide**)
- IT 106-51-4P, 1,4-Benzoquinone, preparation 120-80-9P, Catechol,
 preparation 123-31-9P, Hydroquinone, preparation
 (Cu²⁺-exchanged zeolites as catalysts for phenol hydroxylation
 with **hydrogen peroxide**)
- IT 108-95-2, Phenol, reactions **7722-84-1, Hydrogen**
peroxide, reactions
 (Cu²⁺-exchanged zeolites as catalysts for phenol hydroxylation
 with **hydrogen peroxide**)
- IT 3251-23-8, Copper(II) nitrate
 (in catalyst prepn.; Cu²⁺-exchanged zeolites as catalysts for
 phenol hydroxylation with **hydrogen peroxide**)

L67 ANSWER 3 OF 20 HCA COPYRIGHT 2006 ACS on STN
 140:271376 Catalytic epoxidation process for the manufacture of
 propylene oxide from propylene and oxygen and hydrogen. Cochran,

Robert N.; Balan, Prakash G.; Liepa, Mark A.; Cooker, Bernard (Arco Chemical Technology, L.P., USA). U.S. US 6710194 B1 20040323, 6 pp. (English). CODEN: USXXAM. APPLICATION: US 2003-349655 20030123.

AB Propylene oxide is produced by the liq.-phase epoxidn. reaction of propylene oxygen and hydrogen in contact with a solid epoxidn. **catalyst** (e.g., Pd/TS-1) at elevated temps. and pressures, the reaction conditions being regulated to provide a wt. ratio of dissolved oxygen to dissolved hydrogen in the liq. reaction mixt. of .gtoreq.16 using a fully back-mixed, stirred tank reactor. A reactor schematic and a process flow diagram are presented.

IT **7440-05-3, Palladium**, uses
(**catalytic** epoxidn. process for the manuf. of propylene oxide from propylene and oxygen and hydrogen)

RN 7440-05-3 HCA

CN Palladium (8CI, 9CI) (CA INDEX NAME)

Pd

IT **7782-44-7, Oxygen**, reactions
(**catalytic** epoxidn. process for the manuf. of propylene oxide from propylene and oxygen and hydrogen)

RN 7782-44-7 HCA

CN Oxygen (8CI, 9CI) (CA INDEX NAME)

O=O

IT **1333-74-0, Hydrogen**, reactions
(**catalytic** epoxidn. process for the manuf. of propylene oxide from propylene and oxygen and hydrogen)

RN 1333-74-0 HCA

CN Hydrogen (8CI, 9CI) (CA INDEX NAME)

H-H

IC ICM C07D301-06

INCL 549533000; 549532000

CC 35-2 (Chemistry of Synthetic High Polymers)
Section cross-reference(s): 27, 48, 67

IT Epoxidation **catalysts**
(Pd/TS-1 for the manuf. of propylene oxide from propylene and oxygen and hydrogen)

IT **7440-05-3, Palladium**, uses
(**catalytic** epoxidn. process for the manuf. of propylene oxide from propylene and oxygen and hydrogen)

- IT 115-07-1, Propene, reactions 7782-44-7, Oxygen, reactions
(catalytic epoxidn. process for the manuf. of propylene oxide
from propylene and oxygen and hydrogen)
- IT 1333-74-0, Hydrogen, reactions
(catalytic epoxidn. process for the manuf. of propylene oxide
from propylene and oxygen and hydrogen)
- L67 ANSWER 4 OF 20 HCA COPYRIGHT 2006 ACS on STN
138:304685 Dense-phase epoxidation process and catalysts for the
manufacture of epoxides from olefins and oxygen and hydrogen in the
presence of carbon dioxide solvent. Hancu, Dan; Beckman, Eric John;
Danciu, Tiberiu (Arco Chemical Technology, L.P., USA). U.S. Pat.
Appl. Publ. US 2003073856 A1 20030417, 4 pp. (English). CODEN:
USXXCO. APPLICATION: US 2001-981198 20011016.
- AB Epoxides (e.g., propylene oxide) are manufd. in high yield and
selectivity by the reaction of hydrogen, oxygen, and an olefin
(e.g., propylene) over a solid epoxidn. catalyst such as a
Platinum-Group metal on titanium or vanadium silicalite (e.g., Pd/
TS-1), the reaction being carried out in a carbon
dioxide solvent at conditions effective to provide a dense-phase
reaction mixt.
- IT 7440-05-3, Palladium, uses
(catalyst on titanium silicalite for the manuf. of
epoxides from olefins and oxygen and hydrogen in the presence of
carbon dioxide solvent)
- RN 7440-05-3 HCA
CN Palladium (8CI, 9CI) (CA INDEX NAME)
- Pd
- IT 1333-74-0, Hydrogen, uses
(dense-phase epoxidn. process and catalysts for the manuf. of
epoxides from olefins and oxygen and hydrogen in the presence of
carbon dioxide solvent)
- RN 1333-74-0 HCA
CN Hydrogen (8CI, 9CI) (CA INDEX NAME)
- H-H
- IT 7782-44-7, Oxygen, reactions
(dense-phase epoxidn. process and catalysts for the manuf. of
epoxides from olefins and oxygen and hydrogen in the presence of
carbon dioxide solvent)
- RN 7782-44-7 HCA
CN Oxygen (8CI, 9CI) (CA INDEX NAME)

O=O

- IC ICM C07D301-06
INCL 549533000
CC 35-2 (Chemistry of Synthetic High Polymers)
Section cross-reference(s): 27, 48, 67
IT **Platinum**-group metals
(**catalysts** on titanium or vanadium silicalite for the
manuf. of epoxides from olefins and oxygen and hydrogen in the
presence of carbon dioxide solvent)
IT Epoxidation **catalysts**
(dense-phase; **Platinum**-Group metal on titanium or
vanadium silicalite in a dense-phase epoxidn. process for the
manuf. of epoxides from olefins and oxygen and hydrogen in the
presence of carbon dioxide solvent)
IT Titanium silicalite
(**support**; **catalysts** with **Pt**-Group
metals for the manuf. of epoxides from olefins and oxygen and
hydrogen in the presence of carbon dioxide solvent)
IT Silicalites (zeolites)
(vanadium silicalite, **support**; **catalysts** with
Pt-Group metals for the manuf. of epoxides from olefins
and oxygen and hydrogen in the presence of carbon dioxide
solvent)
IT 7440-05-3, **Palladium**, uses
(**catalyst** on titanium silicalite for the manuf. of
epoxides from olefins and oxygen and hydrogen in the presence of
carbon dioxide solvent)
IT 1333-74-0, Hydrogen, uses
(dense-phase epoxidn. process and **catalysts** for the manuf. of
epoxides from olefins and oxygen and hydrogen in the presence of
carbon dioxide solvent)
IT 7782-44-7, Oxygen, reactions
(dense-phase epoxidn. process and **catalysts** for the manuf. of
epoxides from olefins and oxygen and hydrogen in the presence of
carbon dioxide solvent)
- L67 ANSWER 5 OF 20 HCA COPYRIGHT 2006 ACS on STN
138:39702 Direct epoxidation process using a mixed catalyst system with
a buffer which is useful for the manufacture of propylene oxide.
Grey, Roger A.; Jones, C. Andrew (Arco Chemical Technology L.P.,
USA). U.S. US 6498259 B1 20021224, 7 pp. (English). CODEN:
USXXAM. APPLICATION: US 2001-46502 20011019.
AB The liq.-phase epoxidn. reaction of an olefin (e.g., propylene) with
hydrogen and oxygen in the presence of a catalyst mixt. contg. a
titanium zeolite and a supported **catalyst**
(e.g., **Pd**/niobia) surprisingly produces epoxides (e.g.,

propylene oxide) contg. less ring-opened products such as glycols when performed in the presence of a buffer (e.g., cesium phosphate). This is surprising because a typical palladium on **titanium zeolite** catalyst is little effected by the presence of a buffer and the use of a buffer also typically improves the activity of the process.

IT 7440-05-3, **Palladium**, uses
(epoxidn. **catalysts** with titanosilicate zeolites in a direct epoxidn. process with a buffer which is useful for the manuf. of propylene oxide)

RN 7440-05-3 HCA

CN Palladium (8CI, 9CI) (CA INDEX NAME)

Pd

IT 7782-44-7, **Oxygen**, reactions
(in a direct epoxidn. process using a mixed catalyst system with a buffer which is useful for the manuf. of propylene oxide)

RN 7782-44-7 HCA

CN Oxygen (8CI, 9CI) (CA INDEX NAME)

O=O

IT 1333-74-0, **Hydrogen**, reactions
(in a direct epoxidn. process using a mixed catalyst system with a buffer which is useful for the manuf. of propylene oxide)

RN 1333-74-0 HCA

CN Hydrogen (8CI, 9CI) (CA INDEX NAME)

H-H

IC ICM C07D301-06

INCL 549533000; 549532000; 549523000

CC 35-2 (Chemistry of Synthetic High Polymers)

Section cross-reference(s): 27, 48, 67

IT Epoxidation catalysts

(**titanium zeolites** and supported catalysts in a direct epoxidn. process with a buffer which is useful for the manuf. of propylene oxide)

IT 7440-05-3, **Palladium**, uses 7440-57-5, **Gold**, uses
(epoxidn. **catalysts** with titanosilicate zeolites in a direct epoxidn. process with a buffer which is useful for the manuf. of propylene oxide)

IT 7782-44-7, **Oxygen**, reactions
(in a direct epoxidn. process using a mixed catalyst system with

- a buffer which is useful for the manuf. of propylene oxide)
- IT 1333-74-0, Hydrogen, reactions
(in a direct epoxidn. process using a mixed catalyst system with
a buffer which is useful for the manuf. of propylene oxide)
- L67 ANSWER 6 OF 20 HCA COPYRIGHT 2006 ACS on STN
137:185989 Direct liquid-phase epoxidation process using a mixed
catalyst system of **palladium** on a niobium oxide
support and containing a **titanium zeolite**.
Grey, Roger A. (Arco Chemical Technology, L.P., USA). U.S. US
6441204 B1 20020827, 5 pp. (English). CODEN: USXXAM. APPLICATION:
US 2001-45888 20011019.
- AB A liq.-phase process for epoxidizing an olefin with hydrogen and
oxygen in the presence of a catalyst mixt. comprises a
titanium zeolite (e.g., TS-1)
and a **supported catalyst** comprising
palladium on niobium-contg. support (e.g., Nb2O5). The
process is highly selective and productive for transforming olefins
(e.g., propylene) into epoxides (e.g., propylene oxide) in the
liq.-phase reaction of an olefin, hydrogen, and oxygen.
- IT 7440-05-3, Palladium, uses
(direct liq.-phase epoxidn. process using a mixed
catalyst system of **palladium** on a niobium oxide
support and contg. a **titanium zeolite**)
- RN 7440-05-3 HCA
CN Palladium (8CI, 9CI) (CA INDEX NAME)
- Pd
- IT 7782-44-7, Oxygen, reactions
(in a direct liq.-phase epoxidn. process using a mixed
catalyst system of **palladium** on a niobium oxide
support and contg. a **titanium zeolite**)
- RN 7782-44-7 HCA
CN Oxygen (8CI, 9CI) (CA INDEX NAME)
- O=O
- IT 1333-74-0, Hydrogen, reactions
(in a direct liq.-phase epoxidn. process using a mixed
catalyst system of **palladium** on a niobium oxide
support and contg. a **titanium zeolite**)
- RN 1333-74-0 HCA
CN Hydrogen (8CI, 9CI) (CA INDEX NAME)

H-H

IC ICM C07D301-06

INCL 549533000

CC 35-2 (Chemistry of Synthetic High Polymers)

Section cross-reference(s): 27, 48, 67

IT Alcohols, uses

(C1-4, solvents; in a direct liq.-phase epoxidn. process using a mixed **catalyst** system of **palladium** on a niobium oxide support and contg. a **titanium zeolite**)

IT Hydrocarbons, uses

(C1-6, carriers; in a direct liq.-phase epoxidn. process using a mixed **catalyst** system of **palladium** on a niobium oxide support and contg. a **titanium zeolite**)

IT Titanium silicalite

(TS-1; direct liq.-phase epoxidn. process using a mixed **catalyst** system of **palladium** on a niobium oxide support and contg. a **titanium zeolite**)

IT Epoxidation catalysts

(direct liq.-phase epoxidn. process using a mixed **catalyst** system of **palladium** on a niobium oxide support and contg. a **titanium zeolite**)

IT Titanosilicate zeolites

(direct liq.-phase epoxidn. process using a mixed **catalyst** system of **palladium** on a niobium oxide support and contg. a **titanium zeolite**)

IT Epoxides

(direct liq.-phase epoxidn. process using a mixed **catalyst** system of **palladium** on a niobium oxide support and contg. a **titanium zeolite**)

IT Alkenes, reactions

(direct liq.-phase epoxidn. process using a mixed **catalyst** system of **palladium** on a niobium oxide support and contg. a **titanium zeolite**)

IT Buffers

(in a direct liq.-phase epoxidn. process using a mixed **catalyst** system of **palladium** on a niobium oxide support and contg. a **titanium zeolite**)

IT 69089-35-6, Cesium phosphate

(buffer; in a direct liq.-phase epoxidn. process using a mixed **catalyst** system of **palladium** on a niobium oxide support and contg. a **titanium zeolite**)

IT 74-98-6, Propane, uses 124-38-9, Carbon dioxide, uses 7440-01-9,

- Neon, uses 7440-37-1, Argon, uses 7440-59-7, Helium, uses 7727-37-9, Nitrogen, uses (carrier; in a direct liq.-phase epoxidn. process using a mixed **catalyst** system of **palladium** on a niobium oxide support and contg. a **titanium zeolite**)
- IT 1313-96-8, Dinioibium pentoxide 7440-05-3, Palladium, uses (direct liq.-phase epoxidn. process using a mixed **catalyst** system of **palladium** on a niobium oxide support and contg. a **titanium zeolite**)
- IT 75-56-9P, Propylene oxide, preparation (direct liq.-phase epoxidn. process using a mixed **catalyst** system of **palladium** on a niobium oxide support and contg. a **titanium zeolite**)
- IT 7782-44-7, Oxygen, reactions (in a direct liq.-phase epoxidn. process using a mixed **catalyst** system of **palladium** on a niobium oxide support and contg. a **titanium zeolite**)
- IT 1333-74-0, Hydrogen, reactions (in a direct liq.-phase epoxidn. process using a mixed **catalyst** system of **palladium** on a niobium oxide support and contg. a **titanium zeolite**)
- IT 7732-18-5, Water, uses (solvent; in a direct liq.-phase epoxidn. process using a mixed **catalyst** system of **palladium** on a niobium oxide support and contg. a **titanium zeolite**)
- IT 115-07-1, Propene, reactions (solvent; in a direct liq.-phase epoxidn. process using a mixed **catalyst** system of **palladium** on a niobium oxide support and contg. a **titanium zeolite**)
- IT 7631-86-9, Silica, uses (support; direct liq.-phase epoxidn. process using a mixed **catalyst** system of **palladium** on a niobium oxide support and contg. a **titanium zeolite**)

L67 ANSWER 7 OF 20 HCA COPYRIGHT 2006 ACS on STN

137:6577 Direct alkene epoxidation process using **platinum** -group-metal **catalysts** and carbonate modifiers. Hancu, Dan (Arco Chemical Technology, L.P., USA). U.S. US 6399794 B1 20020604, 5 pp. (English). CODEN: USXXAM. APPLICATION: US 2001-998939 20011115.

AB A process for epoxidizing an olefin (e.g., propylene) with hydrogen and oxygen in the presence of a modifier and a catalyst comprising a noble metal (e.g., Pd) and a **titanium zeolite** is described, which catalyst uses a modifier which is: (a) calcium carbonate in the presence of carbon dioxide; or (b) ammonium bicarbonate. The process results in increased catalyst activity, selectivity to epoxide (e.g., propylene oxide), and increased catalyst life.

IT 7440-05-3, Palladium, uses
(direct alkene epoxidn. process using **platinum**
-group-metal **catalysts** and carbonate modifiers)

RN 7440-05-3 HCA

CN Palladium (8CI, 9CI) (CA INDEX NAME)

Pd

IT 7782-44-7, Oxygen, reactions
(direct alkene epoxidn. process using **platinum**
-group-metal **catalysts** and carbonate modifiers)

RN 7782-44-7 HCA

CN Oxygen (8CI, 9CI) (CA INDEX NAME)

O=O

IT 1333-74-0, Hydrogen, reactions
(direct alkene epoxidn. process using **platinum**
-group-metal **catalysts** and carbonate modifiers)

RN 1333-74-0 HCA

CN Hydrogen (8CI, 9CI) (CA INDEX NAME)

H-H

IC ICM C07D301-06

INCL 549533000

CC 35-2 (Chemistry of Synthetic High Polymers)
Section cross-reference(s): 27, 48, 67

IT Platinum-group metals
(direct alkene epoxidn. process using **platinum**
-group-metal **catalysts** and carbonate modifiers)

IT Epoxides
(direct alkene epoxidn. process using **platinum**
-group-metal **catalysts** and carbonate modifiers)

IT Alkenes, reactions
(direct alkene epoxidn. process using **platinum**
-group-metal **catalysts** and carbonate modifiers)

IT Titanium silicalite
Titanosilicate zeolites
(direct alkene epoxidn. process using **platinum**
-group-metal **catalysts** and carbonate modifiers and)

IT Epoxidation **catalysts**
(**platinum**-group-metal **catalysts** and carbonate
modifiers for the conversion of alkenes with oxygen and hydrogen
into epoxides)

- IT 124-38-9, Carbon dioxide, uses 471-34-1, Calcium carbonate, uses 1066-33-7, Ammonium bicarbonate **7440-05-3**, Palladium, uses (direct alkene epoxidn. process using **platinum** -group-metal **catalysts** and carbonate modifiers)
- IT 75-56-9P, Methyloxirane, preparation (direct alkene epoxidn. process using **platinum** -group-metal **catalysts** and carbonate modifiers)
- IT 115-07-1, Propene, reactions **7782-44-7**, Oxygen, reactions (direct alkene epoxidn. process using **platinum** -group-metal **catalysts** and carbonate modifiers)
- IT **1333-74-0**, Hydrogen, reactions (direct alkene epoxidn. process using **platinum** -group-metal **catalysts** and carbonate modifiers)
- IT 64-17-5, Ethanol, uses 67-56-1, Methanol, uses 67-63-0, 2-Propanol, uses 75-65-0, tert-Butanol, uses 7732-18-5, Water, uses (solvent; direct alkene epoxidn. process using **platinum** -group-metal **catalysts** and carbonate modifiers)

L67 ANSWER 8 OF 20 HCA COPYRIGHT 2006 ACS on STN

136:391481 An ESR study of titanium-silicalite in presence of **H2O2**. Bonoldi, L.; Busetto, C.; Congiu, A.; Marra, G.; Ranghino, G.; Salvalaggio, M.; Spano, G.; Giamello, E. (Enichem Novara, Novara, 28100, Italy). Spectrochimica Acta, Part A: Molecular and Biomolecular Spectroscopy, 58A(6), 1143-1154 (English) 2002. CODEN: SAMCAS. ISSN: 1386-1425. Publisher: Elsevier Science B.V..

AB The interaction of **H2O2** with **TS-1** has been investigated by the ESR technique. A well manufd. **TS-1** has been used, where the presence of extra-structural titanium can be excluded. The two main signals obsd. are attributed to oxygen radical species coordinated on structural titanium sites, and the relevant effect of water presence in the paramagnetic complex is discussed. A comparison is performed with **O2** -/Ti species in **TS-1** obtained by redn./re-oxidn. procedures of Ti(IV). Moreover, some possible structural configurations of the paramagnetic sites are proposed, for two of which ab initio calcn. yield gz values quite close to the exptl. ones.

IT **7722-84-1**, Hydrogen peroxide, processes (ESR study of titanium-silicalite interaction with **H2O2**)

RN 7722-84-1 HCA

CN Hydrogen peroxide (**H2O2**) (9CI) (CA INDEX NAME)

HO-OH

- CC 67-1 (Catalysis, Reaction Kinetics, and Inorganic Reaction Mechanisms)
Section cross-reference(s): 77
- ST titanium silicalite interaction **hydrogen peroxide**
ESR; water titanium silicalite interaction **hydrogen peroxide** ESR
- IT ESR (electron spin resonance)
g-factor (Lande)
(ESR study of titanium-silicalite interaction with **H2O2**)
- IT Titanium silicalite
(**TS-1**; ESR study of titanium-silicalite interaction with **H2O2**)
- IT **7722-84-1, Hydrogen peroxide, processes**
(ESR study of titanium-silicalite interaction with **H2O2**)
- IT 7732-18-5, Water, uses
(ESR study of titanium-silicalite interaction with **H2O2** in presence of)
- L67 ANSWER 9 OF 20 HCA COPYRIGHT 2006 ACS on STN
136:327376 Direct alkene epoxidation process and apparatus. Balan, Prakash G. (Arco Chemical Technology, L.P., USA). U.S. US 6376686 B1 20020423, 4 pp. (English). CODEN: USXXAM. APPLICATION: US 2001-946321 20010905.
- AB An olefin epoxidn. process is presented which comprises reacting an olefin (e.g., propylene), oxygen, and hydrogen in a liq. medium in the presence of an epoxidn. **catalyst** (e.g., **Pd** on **TS-1** zeolite) in a reactor system comprising a tank, a tube, a plurality of impellers, and a means for inhibiting flow. The reactor system facilitates transfer of the hydrogen and oxygen to the liq. medium.
- IT **7782-44-7, Oxygen, reactions**
(direct alkene epoxidn. process and app. for the manuf. of epoxides using)
- RN 7782-44-7 HCA
- CN Oxygen (8CI, 9CI) (CA INDEX NAME)
- O=O
- IT **1333-74-0, Hydrogen, reactions**
(direct alkene epoxidn. process and app. for the manuf. of epoxides using)
- RN 1333-74-0 HCA
- CN Hydrogen (8CI, 9CI) (CA INDEX NAME)

H-H

IC ICM C07D301-06

INCL 549532000

CC 45-4 (Industrial Organic Chemicals, Leather, Fats, and Waxes)
Section cross-reference(s): 27, 47, 48IT Epoxidation **catalysts**
(**Pd** on a **TS-1** zeolite in a direct
alkene epoxidn. process and app. for the manuf. of epoxides)IT Titanium silicalite
(**TS-1**, support; epoxidn. **catalyst**
with **Pd** in a direct alkene epoxidn. process and app.
for the manuf. of epoxides)IT 115-07-1, Propene, reactions **7782-44-7**, Oxygen, reactions
(direct alkene epoxidn. process and app. for the manuf. of
epoxides using)IT **1333-74-0**, Hydrogen, reactions
(direct alkene epoxidn. process and app. for the manuf. of
epoxides using)

L67 ANSWER 10 OF 20 HCA COPYRIGHT 2006 ACS on STN

136:91464 Redox behavior and selective oxidation properties of
mesoporous titano- and zirconsilicate MCM-41 molecular sieves.
Chaudhari, K.; Bal, R.; Srinivas, D.; Chandwadkar, A. J.;
Sivasanker, S. (Catalysis Division, National Chemical Laboratory,
Pune, 411008, India). Microporous and Mesoporous Materials,
50(2-3), 209-218 (English) 2001. CODEN: MIMMFJ. ISSN: 1387-1811.
Publisher: Elsevier Science B.V..AB Mesoporous titano- and zirconsilicate mol. sieves, Ti-MCM-41 and
Zr-MCM-41, resp., with Si/M ratios in the range from 11 to 96 (M=Ti
or Zr), have been synthesized by the hydrothermal method and
characterized by XRD, XRF, N₂ adsorption and diffusive reflectance
UV-Vis (DRUV-Vis), FT-IR and ESR spectroscopic techniques. The
redox behavior and selective oxidn. properties of these materials
have been investigated. ESR of samples reduced with LiAlH₄ (298 K)
and H₂ (673-873 K) reveals two types of metal ion species:
species I' located inside the pore walls and species I'' located at
the pore surface. The reduced species I'' are highly reactive
towards oxygen and form M(O₂-.cntdot.) radicals. The M(
O₂-.cntdot.) radicals were also obsd. when the samples were
reacted with aq. H₂O₂ or tert-butylhydroperoxide (TBHP).
ESR studies reveal that Ti-MCM-41 is easier to reduce and reoxidize
than Zr-MCM-41. The DRUV-Vis spectra are consistent with a monoa.
dispersion of the metal ions. In the samples with high metal
loading the presence of a nanocryst. metal oxide phase cannot be
ruled out. Both Ti-MCM-41 and Zr-MCM-41 catalyze the hydroxylation

of 1-naphthol with aq. **H2O2** and the epoxidn. of norbornylene with TBHP.

CC 67-2 (Catalysis, Reaction Kinetics, and Inorganic Reaction Mechanisms)

Section cross-reference(s): 24, 25, 73, 77

IT **Zeolite MCM-41**

(Ti-MCM-41, Zr-MCM-41; redox behavior and selective oxidn. properties of mesoporous titano- and zirconsilicate MCM-41 mol. sieves)

L67 ANSWER 11 OF 20 HCA COPYRIGHT 2006 ACS on STN

135:195939 Direct epoxidation process of olefins using **palladium**-titanosilicate **catalyst** containing gold promotor.

Jewson, Jennifer D.; Jones, C. Andrew; Dessau, Ralph M. (Arco Chemical Technology, L.P., USA). PCT Int. Appl. WO 2001062380 A1 20010830, 14 pp. DESIGNATED STATES: W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG, TR. (English). CODEN: PIXXD2. APPLICATION: WO 2001-US1453 20010117. PRIORITY: US 2000-507842 20000222.

AB Title process, exhibiting high selectivity and productivity, comprises reacting an olefin, hydrogen, and oxygen in the presence of a catalyst contg. **titanium zeolite**, **palladium**, and a gold promoter. Thus, propylene was epoxidized in the presence of 5% **Pd**-contg. **catalyst** prepd. from **TS-1** (titanium silicalite), $\text{Pd}(\text{NH}_3)_4(\text{NO}_3)_2$, and AuCl_3 to give propylene oxide equiv. products (POE: propylene oxide, propylene glycol, dipropylene glycol, and acetol) with productivity of 0.017 g POE/g cat/h and propylene to POE selectivity 98% as compared with productivity 0.0065 and selectivity 85% without AuCl_3 .

IT **7440-05-3, Palladium**, uses

(**catalyst**; direct epoxidn. process of olefins using **palladium**-titanosilicate **catalyst** contg. gold promoter)

RN 7440-05-3 HCA

CN Palladium (8CI, 9CI) (CA INDEX NAME)

Pd

IT **1333-74-0, Hydrogen**, reactions **7782-44-7, Oxygen**, reactions

(direct epoxidn. process of olefins using **palladium**
-titanosilicate **catalyst** contg. gold promoter)

RN 1333-74-0 HCA

CN Hydrogen (8CI, 9CI) (CA INDEX NAME)

H-H

RN 7782-44-7 HCA

CN Oxygen (8CI, 9CI) (CA INDEX NAME)

O=O

IC ICM B01J021-16

ICS B01J023-52; B01J023-66; B01J029-04; C07D301-06; C07D301-10

CC 35-2 (Chemistry of Synthetic High Polymers)

Section cross-reference(s): 67

ST olefin epoxidn **palladium** titanosilicate **catalyst**

gold promoter; propylene epoxidn **palladium** titanosilicate

catalyst gold promoter

IT Hydrocarbons, uses

(C1-8, carrier gas; direct epoxidn. process of olefins using
palladium-titanosilicate **catalyst** contg. gold
promoter)

IT Titanium silicalite

(**TS-1**, catalyst; direct epoxidn. process of
olefins using **palladium**-titanosilicate **catalyst**
contg. gold promoter)

IT Titanosilicate zeolites

Zeolites (synthetic), uses

(catalyst; direct epoxidn. process of olefins using
palladium-titanosilicate **catalyst** contg. gold
promoter)

IT Epoxidation

Epoxidation catalysts

(direct epoxidn. process of olefins using **palladium**
-titanosilicate **catalyst** contg. gold promoter)

IT Epoxides

(direct epoxidn. process of olefins using **palladium**
-titanosilicate **catalyst** contg. gold promoter)

IT Alkenes, reactions

(direct epoxidn. process of olefins using **palladium**
-titanosilicate **catalyst** contg. gold promoter)

IT Group IB element halides

(gold halides; direct epoxidn. process of olefins using
palladium-titanosilicate **catalyst** contg. gold
promoter)

- IT Platinum-group metal compounds
Transition metal halides
(**palladium** halides, **catalyst**; direct epoxidn.
process of olefins using **palladium**-titanosilicate
catalyst contg. gold promoter)
- IT 124-38-9, Carbon dioxide, uses 7440-01-9, Neon, uses 7440-37-1,
Argon, uses 7440-59-7, Helium, uses 7727-37-9, Nitrogen, uses
(carrier gas; direct epoxidn. process of olefins using
palladium-titanosilicate **catalyst** contg. gold
promoter)
- IT 7440-05-3, **Palladium**, uses 10102-05-3,
Palladium nitrate 13566-03-5, **Palladium** sulfate
13601-08-6
(**catalyst**; direct epoxidn. process of olefins using
palladium-titanosilicate **catalyst** contg. gold
promoter)
- IT 37187-64-7, Gold cyanide 54182-83-1, Gold hydroxide 126549-44-8,
Gold sulfide
(direct epoxidn. process of olefins using **palladium**
-titanosilicate **catalyst** contg. gold promoter)
- IT 75-56-9P, Propylene oxide, preparation
(direct epoxidn. process of olefins using **palladium**
-titanosilicate **catalyst** contg. gold promoter)
- IT 115-07-1, Propylene, reactions 1333-74-0, Hydrogen,
reactions 7782-44-7, Oxygen, reactions
(direct epoxidn. process of olefins using **palladium**
-titanosilicate **catalyst** contg. gold promoter)
- IT 7440-57-5, Gold, uses 13453-07-1, Gold trichloride
(promoter; direct epoxidn. process of olefins using
palladium-titanosilicate **catalyst** contg. gold
promoter)
- IT 64-17-5, Ethanol, uses 67-56-1, Methanol, uses 67-63-0,
Isopropanol, uses 75-65-0, tert-Butanol, uses 7732-18-5, Water,
uses
(solvent; direct epoxidn. process of olefins using
palladium-titanosilicate **catalyst** contg. gold
promoter)

L67 ANSWER 12 OF 20 HCA COPYRIGHT 2006 ACS on STN

133:225066 Molecular sieves for decontamination of gases. Cruickshank,
Graeme Duncan; Stoddart, Barry; Davison, Gordon Robert (The Procter
& Gamble Company, USA). PCT Int. Appl. WO 2000051713 A1 20000908,
19 pp. DESIGNATED STATES: W: AE, AL, AM, AT, AU, AZ, BA, BB,
BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI,
GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG,
KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN,
MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ,
TM, TR, TT, TZ, UA, UG, US, VZ, VN, YU, ZA, ZW, AM, AZ, BY, KG,
KZ, MD, RU, TJ,

TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG.
(English). CODEN: PIXXD2. APPLICATION: WO 2000-US4907 20000225.
PRIORITY: GB 1999-4440 19990227.

AB Large-pore mol. sieves contg. a d.pi.-donor guest material and having a pore diam. >4 .ANG., esp. M41S and MCM-41 zeolites, are used as agents for non-catalytic sorptive decontamination of a non-.pi. acceptor gas or gas mixts. contg. .pi.-acceptor gas pollutants. Preferred guest materials are Group IB elements, esp. Cu and Ag, and Group VIII elements. The methods, compns. and devices can be used in decontamination of a variety of non-.pi. acceptor gases or gas mixts., e.g., air, O₂, N₂, CO₂, H₂, inert gases, satd. hydrocarbon gases and their mixts., contg. a range of .pi.-acceptor gas pollutants, e.g., CO, NO_x, SO_x, ethylene and their mixts.

IT 7440-02-0, Nickel, uses 7440-05-3, Palladium, uses 7440-06-4, Platinum, uses
(mol. sieve sorbents contg.; mol. sieve sorbents for decontamination of gases)

RN 7440-02-0 HCA

CN Nickel (8CI, 9CI) (CA INDEX NAME)

Ni

RN 7440-05-3 HCA

CN Palladium (8CI, 9CI) (CA INDEX NAME)

Pd

RN 7440-06-4 HCA

CN Platinum (8CI, 9CI) (CA INDEX NAME)

Pt

IT 1333-74-0P, Hydrogen, processes
7782-44-7P, Oxygen, processes
(mol. sieve sorbents for decontamination of gases)

RN 1333-74-0 HCA

CN Hydrogen (8CI, 9CI) (CA INDEX NAME)

H-H

RN 7782-44-7 HCA

CN Oxygen (8CI, 9CI) (CA INDEX NAME)

O=O

- IC ICM B01D053-02
ICS B01J020-18
- CC 48-1 (Unit Operations and Processes)
Section cross-reference(s): 49, 51, 59
- IT **Air** purification
Molecular sieves
Sorbents
(mol. sieve sorbents for decontamination of gases)
- IT **7440-02-0**, Nickel, uses **7440-05-3**, Palladium, uses
7440-06-4, Platinum, uses 7440-16-6, Rhodium, uses
7440-22-4, Silver, uses 7440-50-8, Copper, uses
(mol. sieve sorbents contg.; mol. sieve sorbents for
decontamination of gases)
- IT 124-38-9P, Carbon dioxide, processes **1333-74-0P**,
Hydrogen, processes 7727-37-9P, Nitrogen,
processes **7782-44-7P**, **Oxygen, processes**
(mol. sieve sorbents for decontamination of gases)
- IT 7439-89-6, Iron, uses 7439-95-4, Magnesium, uses 7439-96-5,
Manganese, uses 7440-32-6, **Titanium**, uses 7440-48-4,
Cobalt, uses 7440-55-3, Gallium, uses 7440-66-6, Zinc, uses
(silicoaluminophosphate **zeolites** contg.; mol. sieve
sorbents for decontamination of gases)
- L67 ANSWER 13 OF 20 HCA COPYRIGHT 2006 ACS on STN
132:336090 Process of epoxidizing olefins using noble metal-modified
titanium or vanadium **zeolite** catalysts. Grey,
Roger A. (Arco Chemical Technology, L.P., USA). U.S. US 6063942 A
20000516, 5 pp. (English). CODEN: USXXAM. APPLICATION: US
1999-406865 19990927.
- AB Title process for epoxidizing an olefin comprises reacting an olefin
with **H2** and **O2** in a reaction zone in the
presence of a noble metal-contg. titanium or vanadium silicalite
catalyst prepd. by contacting the vanadium or titanium silicalite
slurry with an ion exchangeable noble metal complex without drying
or calcining. Thus, 1:1:4 **H2**, **O2** and propylene
were reacted in the presence of a mixt. of palladium bromide,
TS 1 (titanium silicalite) slurried in deionized
water, showing 2700 ppm propylene oxide at the peak and propylene
oxide/propylene glycol 2 in vapor phase measured by GC.
- IT **7440-05-3**, Palladium, uses
(process of epoxidizing olefins using noble metal-modified
titanium or vanadium **zeolite** catalysts)
- RN 7440-05-3 HCA
CN Palladium (8CI, 9CI) (CA INDEX NAME)

Pd

IC ICM C07D301-03

ICS C07D301-06

INCL 549523000

CC 45-4 (Industrial Organic Chemicals, Leather, Fats, and Waxes)

Section cross-reference(s): 67

ST olefin epoxidn noble metal **titanium zeolite**
catalyst; vanadium zeolite noble metal catalyst epoxidn; propylene
oxide prepn titanium silicalite **palladium catalyst**

IT Titanium silicalite

(**TS 1**; process of epoxidizing olefins using
noble metal-modified **titanium** or vanadium
zeolite catalysts)

IT Epoxidation

Epoxidation catalysts

(process of epoxidizing olefins using noble metal-modified
titanium or vanadium **zeolite** catalysts)

IT Noble metals

Titanosilicate zeolites

(process of epoxidizing olefins using noble metal-modified
titanium or vanadium **zeolite** catalysts)

IT Epoxides

(process of epoxidizing olefins using noble metal-modified
titanium or vanadium **zeolite** catalysts)

IT Alkenes, reactions

(process of epoxidizing olefins using noble metal-modified
titanium or vanadium **zeolite** catalysts)

IT Zeolites (synthetic), uses

(vanadosilicate; process of epoxidizing olefins using noble
metal-modified **titanium** or vanadium **zeolite**
catalysts)

IT **7440-05-3**, Palladium, uses 13444-94-5, Palladium dibromide

13601-08-6, Tetraamminepalladium dinitrate

(process of epoxidizing olefins using noble metal-modified
titanium or vanadium **zeolite** catalysts)

IT 75-56-9P, Propylene oxide, preparation

(process of epoxidizing olefins using noble metal-modified
titanium or vanadium **zeolite** catalysts)

IT 115-07-1, Propylene, reactions

(process of epoxidizing olefins using noble metal-modified
titanium or vanadium **zeolite** catalysts)

L67 ANSWER 14 OF 20 HCA COPYRIGHT 2006 ACS on STN

131:351165 Synthesis of propylene oxide from propylene, oxygen and
hydrogen catalyzed by **palladium-platinum**

-containing titanium silicalite. Laufer, W.; Meiers, R.; Holderich, W. F. (Department of Chemical Technology and Heterogeneous Catalysis, University of Technology RWTH Aachen, Aachen, 52074, Germany). Proceedings of the International Zeolite Conference, 12th, Baltimore, July 5-10, 1998, Meeting Date 1998, Volume 2, 1351-1358. Editor(s): Treacy, M. M. J. Materials Research Society: Warrendale, Pa. (English) 1999. CODEN: 68DCAH.

AB **TS-1**-catalysts modified by impregnation with palladium tetraammine and platinum tetrachloride were tested as catalysts for the synthesis of propylene oxide (PO) from propylene, oxygen and hydrogen. The effect of various redn. methods and Pt loading on the catalytic performance and phys. characteristics of the catalysts have been studied. The redn. of the tetraammine ligand under a flow of N₂ at 150.degree.C leads to high PO selectivities and yields. High PO yields were also obtained over a **TS-1** catalyst loaded with 1 wt% Pd and 0.02 wt% Pt and reduced under N₂ at 150.degree.C. Addnl. the PO-yields can be even more increased by addn. of small amts. of salts (halides) to the solvent. This influence was investigated with different salts in various concn. The change of the reaction-procedure from the batch to the semi-continuous manner leads to an increased PO-selectivity. Furthermore, the PO-selectivity can be improved by addn. of polyfluorinated hydrocarbons as solvent to the reaction mixt.

IT **7440-05-3**, Palladium, uses **7440-06-4**, Platinum, uses
(prepn. of propylene oxide from propylene, oxygen and hydrogen
catalyzed by **palladium-platinum**
-contg. titanium silicalite)

RN 7440-05-3 HCA
CN Palladium (8CI, 9CI) (CA INDEX NAME)

Pd

RN 7440-06-4 HCA
CN Platinum (8CI, 9CI) (CA INDEX NAME)

Pt

IT **1333-74-0**, Hydrogen, reactions **7782-44-7**, Oxygen, reactions
(prepn. of propylene oxide from propylene, oxygen and hydrogen
catalyzed by **palladium-platinum**
-contg. titanium silicalite)

RN 1333-74-0 HCA
CN Hydrogen (8CI, 9CI) (CA INDEX NAME)

H-H

RN 7782-44-7 HCA
CN Oxygen (8CI, 9CI) (CA INDEX NAME)

O=O

- CC 27-2 (Heterocyclic Compounds (One Hetero Atom))
IT Titanium silicalite
(TS-1; prepn. of propylene oxide from propylene, oxygen and hydrogen **catalyzed** by **palladium-platinum**-contg. titanium silicalite)
IT Epoxidation
Epoxidation catalysts
(prepn. of propylene oxide from propylene, oxygen and hydrogen **catalyzed** by **palladium-platinum**-contg. titanium silicalite)
IT 7440-05-3, Palladium, uses 7440-06-4, Platinum, uses
(prepn. of propylene oxide from propylene, oxygen and hydrogen **catalyzed** by **palladium-platinum**-contg. titanium silicalite)
IT 7647-15-6, Sodium bromide, uses 7722-88-5 7789-39-1, Rubidium bromide 7790-69-4, Lithium nitrate
(prepn. of propylene oxide from propylene, oxygen and hydrogen **catalyzed** by **palladium-platinum**-contg. titanium silicalite)
IT 75-56-9P, Propylene oxide, preparation
(prepn. of propylene oxide from propylene, oxygen and hydrogen **catalyzed** by **palladium-platinum**-contg. titanium silicalite)
IT 115-07-1, Propylene, reactions 1333-74-0, Hydrogen, reactions 7782-44-7, Oxygen, reactions 13601-08-6, Tetraamminepalladium(2+) dinitrate 13933-32-9, Tetraammineplatinum(2+) dichloride
(prepn. of propylene oxide from propylene, oxygen and hydrogen **catalyzed** by **palladium-platinum**-contg. titanium silicalite)

L67 ANSWER 15 OF 20 HCA COPYRIGHT 2006 ACS on STN

131:272326 Process for the preparation of peroxidation products from mixed olefin and paraffin feedstocks. Young, Desmond Austin; Pretorius, Rudolph Johannes; Smit, Franchuan; Kruger, Friedrich Wilhelm Hein; Monkhe, Thabo Vincent (Sasol Technology (Proprietary) Limited, S. Afr.). PCT Int. Appl. WO 9951557 A1 19991014, 23 pp.

DESIGNATED STATES: W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 1999-IB543 19990329. PRIORITY: ZA 1998-2966 19980407.

- AB Epoxides (e.g., propylene oxide) and/or a glycol and/or a glycol alkyl ether is/are prepd. in high yield and selectivity by reacting a mixed olefin and paraffin feedstock (e.g., a propylene and propane mixt.) in the liq. phase with a peroxidn. component (e.g., **hydrogen peroxide**). The paraffin (e.g., propane) remains substantially unreacted.
- IT **7722-84-1, Hydrogen peroxide**, reactions
7782-44-7, Oxygen, reactions
(**process** for the prepn. of peroxidn. products from mixed olefin and paraffin feedstocks)
- RN 7722-84-1 HCA
- CN Hydrogen peroxide (H2O2) (9CI) (CA INDEX NAME)

HO—OH

- RN 7782-44-7 HCA
- CN Oxygen (8CI, 9CI) (CA INDEX NAME)

O=O

- IC ICM C07C029-10
ICS C07C041-03; C07D301-12
- CC 35-2 (Chemistry of Synthetic High Polymers)
Section cross-reference(s): 27, 48
- IT **Peroxides**, reactions
(**process** for the prepn. of peroxidn. products from mixed olefin and paraffin feedstocks using)
- IT 78-84-2 109-67-1, 1-Pentene 115-07-1, 1-Propene, reactions
592-41-6, 1-Hexene, reactions 691-37-2, 4-Methyl-1-pentene
760-20-3, 3-Methyl-1-pentene **7722-84-1, Hydrogen peroxide**, reactions **7782-44-7, Oxygen**, reactions
(**process** for the prepn. of peroxidn. products from mixed olefin and paraffin feedstocks)
- IT 7440-32-6, **Titanium**, uses
(**zeolites**; **process** for the prepn. of peroxidn. products from mixed olefin and paraffin feedstocks)

L67 ANSWER 16 OF 20 HCA COPYRIGHT 2006 ACS on STN

127:150397 Catalytic manufacture of epoxides from olefins, hydrogen and oxygen. Mueller, Ulrich; Grosch, Georg Heinrich; Schulz, Michael; Rieber, Norbert (BASF A.-G., Germany). Ger. Offen. DE 19600709 A1 19970717, 6 pp. (German). CODEN: GWXXBX. APPLICATION: DE 1996-19600709 19960111.

AB In the title process, which gives better reliability and catalyst durability, olefins are **treated** with **H** and **O** (ratio 1:1-10) in inert gases (inert gas-olefin ratio .ltoreq.20:1) at O-olefin (or olefin plus inert hydrocarbon) ratio 1:3-20 in the presence of **zeolitic Ti** or **V** silicates contg. 0.1-20% Pt-group metal. Passing a mixt. of C3H6 1.3, H 2, O 9.5, and N 0.5 L/h into 1730 mL MeOH contg. 0.76 g Ti silicate contg. 0.49% Pd at 50.degree./4 bar gave an offgas contg. 0.06% propylene oxide after 12 h.

IT **7440-05-3, Palladium**, uses **7440-06-4, Platinum**, uses (catalytic manuf. of epoxides from olefins, hydrogen and oxygen)

RN 7440-05-3 HCA

CN Palladium (8CI, 9CI) (CA INDEX NAME)

Pd

RN 7440-06-4 HCA

CN Platinum (8CI, 9CI) (CA INDEX NAME)

Pt

IT **1333-74-0, Hydrogen, processes**

(catalytic manuf. of epoxides from olefins, hydrogen and oxygen)

RN 1333-74-0 HCA

CN Hydrogen (8CI, 9CI) (CA INDEX NAME)

H-H

IT **7782-44-7, Oxygen, reactions**

(catalytic manuf. of epoxides from olefins, hydrogen and oxygen)

RN 7782-44-7 HCA

CN Oxygen (8CI, 9CI) (CA INDEX NAME)

O=O

- IC ICM C07D301-08
- ICS C07D303-04; B01J029-89
- ICI B01J029-04, B01J103-40
- CC 45-4 (Industrial Organic Chemicals, Leather, Fats, and Waxes)
Section cross-reference(s): 27, 35, 67
- ST epoxide manuf olefin hydrogen oxygen; catalyst epoxidn olefin
oxygen; propylene oxide manuf hydrogen oxygen; propene epoxidn
hydrogen oxygen; **palladium catalyst** epoxidn;
titanium silicate catalyst epoxidn
- IT **Platinum-group metals**
(**catalytic** manuf. of epoxides from olefins, hydrogen
and oxygen)
- IT 7439-88-5, Iridium, uses 7440-04-2, Osmium, uses **7440-05-3**
, **Palladium**, uses **7440-06-4**, **Platinum**,
uses 7440-16-6, Rhodium, uses 7440-18-8, Ruthenium, uses
12653-89-3, Vanadium silicate 42613-21-8, Titanium silicate
(**catalytic** manuf. of epoxides from olefins, hydrogen
and oxygen)
- IT **1333-74-0, Hydrogen, processes**
(catalytic manuf. of epoxides from olefins, hydrogen and oxygen)
- IT 115-07-1, Propylene, reactions **7782-44-7**, Oxygen,
reactions
(catalytic manuf. of epoxides from olefins, hydrogen and oxygen)
- L67 ANSWER 17 OF 20 HCA COPYRIGHT 2006 ACS on STN
- 124:320125 Manufacture of hydroxylamines from ammonia or corresponding
amines, hydrogen, and oxygen. Mueller, Ulrich; Heineke, Daniel
(BASF A.-G., Germany). Ger. Offen. DE 4435239 A1 19960411, 5 pp.
(German). CODEN: GWXXBX. APPLICATION: DE 1994-4435239 19941004.
- AB Hydroxylamines are produced from NH₃ or corresponding amines,
H₂, and **O₂** by using an oxidn. catalyst based on a
Ti silicate or V silicate with a zeolite structure and contg.
0.01-20 wt.% .gtoreq.1 Pt group metal including Ru, Rh, Pd, Os, Ir,
and Pt. The Pt group metals are present in .gtoreq.2 different
binding energy states. The oxidn. catalyst can also contain Fe, Co,
Ni, Re, Ag, and/or Au. The (Ti and/or V)/[Si + (Ti and/or V)] mol
ratio is (0.01-0.1) : 1. The oxidn. catalyst is prepd. by
impregnation of **zeolitic Ti** silicates or V
silicates with Pt group metal salts, chelate complexes, or carbonyl
complexes and subsequent adjustment of the required distribution of
the binding energy states of the Pt group metals under suitable
reducing or oxidizing conditions.
- IT **7782-44-7, Oxygen, processes**
(hydroxylamine manuf. from ammonia or corresponding amines,
hydrogen, and)
- RN 7782-44-7 HCA
- CN Oxygen (8CI, 9CI) (CA INDEX NAME)

O=O

IT 1333-74-0, **Hydrogen, processes**
(hydroxylamine manuf. from ammonia or corresponding amines,
oxygen, and)
RN 1333-74-0 HCA
CN Hydrogen (8CI, 9CI) (CA INDEX NAME)

H-H

IT 7440-02-0, Nickel, uses 7440-05-3, Palladium, uses
7440-06-4, Platinum, uses
(in oxidn. catalyst for hydroxylamine manuf. from ammonia or
corresponding amines, hydrogen, and oxygen)
RN 7440-02-0 HCA
CN Nickel (8CI, 9CI) (CA INDEX NAME)

Ni

RN 7440-05-3 HCA
CN Palladium (8CI, 9CI) (CA INDEX NAME)

Pd

RN 7440-06-4 HCA
CN Platinum (8CI, 9CI) (CA INDEX NAME)

Pt

IC ICM C01B021-14
ICS B01J029-89; C07C239-08
CC 45-4 (Industrial Organic Chemicals, Leather, Fats, and Waxes)
Section cross-reference(s): 49
IT 7782-44-7, **Oxygen, processes**
(hydroxylamine manuf. from ammonia or corresponding amines,
hydrogen, and)
IT 1333-74-0, **Hydrogen, processes**
(hydroxylamine manuf. from ammonia or corresponding amines,
oxygen, and)
IT 7439-88-5, Iridium, uses 7439-89-6, Iron, uses 7440-02-0
, Nickel, uses 7440-04-2, Osmium, uses 7440-05-3,
Palladium, uses 7440-06-4, Platinum, uses 7440-15-5,
Rhenium, uses 7440-16-6, Rhodium, uses 7440-18-8, Ruthenium,

uses 7440-22-4, Silver, uses 7440-48-4, Cobalt, uses
7440-57-5, Gold, uses
(in oxidn. catalyst for hydroxylamine manuf. from ammonia or
corresponding amines, hydrogen, and oxygen)

IT 12653-89-3, Vanadium silicate 42613-21-8, **Titanium**
silicate
(**zeolitic**; in oxidn. catalyst for hydroxylamine manuf.
from ammonia or corresponding amines, hydrogen, and oxygen)

L67 ANSWER 18 OF 20 HCA COPYRIGHT 2006 ACS on STN
122:88196 Deodorants for indoor **air** purification. Sadakata,
Tomohiko (Babcock Hitachi Kk, Japan). Jpn. Kokai Tokkyo Koho JP
06254140 A2 19940913 Heisei, 6 pp. (Japanese). CODEN: JKXXAF.
APPLICATION: JP 1993-49595 19930310.

AB The deodorants comprise a 1st zeolite support having sp. surface
area .gtoreq.100 m²/g, Si/Al at. ratio .ltoreq.5:1 and totally or
partially cation-exchanged with Cs, Rb, K, and/or Na, and a 2nd
zeolite support having sp. surface area .gtoreq.100 m²/g, Si/Al at.
ratio .gtoreq.5:1 and totally or partially cation-exchanged with H,
Li, Mg, Ca, and/or La, and both zeolite supports being loaded with
.gtoreq.1 transition metals of Ti, V, Cr, Mn, Fe, Co, Ni, Cu, Zn,
Zr, Mo, Ag, Pd, and Pt. The deodorants are durable and effective
for removing NH₃, trimethylamine, Me mercaptan, di-Me sulfide, etc.
from odorous **air** in closed rooms, toilets or offices.

IT 7440-02-0, **Nickel**, processes 7440-05-3,
Palladium, processes 7440-06-4, **Platinum**
, processes
(**zeolite supports** loaded with; Deodorants for
indoor **air** purifn.)

RN 7440-02-0 HCA
CN Nickel (8CI, 9CI) (CA INDEX NAME)

Ni

RN 7440-05-3 HCA
CN Palladium (8CI, 9CI) (CA INDEX NAME)

Pd

RN 7440-06-4 HCA
CN Platinum (8CI, 9CI) (CA INDEX NAME)

Pt

IC ICM A61L009-01

- CC 59-6 (Air Pollution and Industrial Hygiene)
ST deodorant zeolite **air** toilet office
IT Zeolites, **processes**
(**H**, Deodorants for indoor **air** purifn.)
IT **Air** purification
(deodorization, in closed rooms or toilets, durable
zeolites-based deodorants for)
IT 74-93-1, Methyl mercaptan, processes 75-18-3, Dimethyl sulfide
75-50-3, Trimethylamine, processes 7664-41-7, Ammonia, processes
(removal of; deodorants for indoor **air** purifn.)
IT 7439-89-6, Iron, processes 7439-91-0, Lanthanum, processes
7439-93-2, Lithium, processes 7439-95-4, Magnesium, processes
7439-96-5, Manganese, processes 7439-98-7, Molybdenum, processes
7440-02-0, Nickel, processes 7440-05-3,
Palladium, processes 7440-06-4, Platinum
, processes 7440-09-7, Potassium, processes 7440-17-7, Rubidium,
processes 7440-22-4, Silver, processes 7440-23-5, Sodium,
processes 7440-32-6, Titanium, processes 7440-46-2,
Cesium, processes 7440-47-3, Chromium, processes 7440-48-4,
Cobalt, processes 7440-50-8, Copper, processes 7440-62-2,
Vanadium, processes 7440-66-6, Zinc, processes 7440-67-7,
Zirconium, processes 7440-70-2, Calcium, processes
(**zeolite supports** loaded with; Deodorants for
indoor **air** purifn.)
- L67 ANSWER 19 OF 20 HCA COPYRIGHT 2006 ACS on STN
118:6689 Hydroxylation of benzene and hexane by oxygen and hydrogen over
palladium-containing titanium silicalites. Tatsumi, T.; Yuasa, K.;
Tominaga, H. (Fac. Eng., Univ. Tokyo, Tokyo, 113, Japan). Journal
of the Chemical Society, Chemical Communications (19), 1446-7
(English) 1992. CODEN: JCCCAT. ISSN: 0022-4936. OTHER SOURCES:
CASREACT 118:6689.
- AB Palladium-contg. **titanium** silicalite **zeolites**
catalyze the hydroxylation of benzene and hexane by **O2-**
H2 under mild conditions to give phenol and hexanols, resp.
IT **7440-05-3, Palladium, uses**
(**catalysts**, contg. titanium silicalites, for
hydroxylation of benzene and hexane)
RN 7440-05-3 HCA
CN Palladium (8CI, 9CI) (CA INDEX NAME)
- Pd
- CC 25-10 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
ST hydroxylation benzene hexane silicalite catalyst; **palladium**
titanium silicalite **catalyst** hydroxylation; phenol;
hexanol

- IT Zeolites, uses
(ATS1, TS1A, and TS1B, **catalysts**, contg.
palladium, for hydroxylation of benzene and hexane)
- IT Hydroxylation **catalysts**
(**palladium**-contg. titanium silicalites, for benzene and
hexane)
- IT Zeolites, uses
(HZSM 5, **catalyst**, contg. **palladium**, for
hydroxylation of benzene and hexane)
- IT 7440-05-3, **Palladium**, uses
(**catalysts**, contg. titanium silicalites, for
hydroxylation of benzene and hexane)

L67 ANSWER 20 OF 20 HCA COPYRIGHT 2006 ACS on STN

53:96971 Original Reference No. 53:17486g-i,17487a

Hydrogenation of shale oil on stationary catalysts. Tsang, Pin-Nan; Wei, Shih-Pin; Lin, Li-Yu; Kuan, Chi; Chou, Fu-Len; Kalechits, I. V. Izvest. Sibir. Otdel. Akad. Nauk S.S.S.R. (No. 2), 81-96 (Unavailable) 1959.

- AB **Hydrogenation** studies were conducted using two shale oils (1.04-1.22% N, 0.32-0.45% S, 0.003-0.017% ash), and a variety of catalysts. The order of descending activity of the catalysts was WS2 > MoS2 > WS2-NiS-Al2O3 > CoMoO4-Al2O3 > MoS2-C. Three types of reactions were studied: (1) reduction of asphaltic compds., S compds., and olefins; (2) reduction of N and O compds.; and (3) **hydrogenation** of aromatic hydrocarbons, hydrocracking of the heavy fraction, and isomerization of normal paraffins. The 1st reaction proceeds easily above 300.degree. without evidence of significant catalyst deactivation. At 400.degree., reduction of N and O compds. and **hydrogenation** of aromatic hydrocarbons takes place. At 400-440.degree., the catalyst gradually becomes deactivated with respect to the **hydrogenation** of aromatic hydrocarbons. Above 400.degree., hydrocracking and isomerization reactions proceed with gradual catalyst deactivation. The group (3) reactions proceed more rapidly at increasing temp. and H pressure (70-260 atm.), and with decreasing space velocity, (0.6-2.4 kg./l./hr.). However, at 460-480.degree. the catalysts slowly become deactivated with respect to all reactions studied. The preferential deactivation at 400-440.degree. is explained by the preferential adsorption of N compds. on the catalyst surface. Hydrotreating of the shale oil is most effective (for runs of 479-1315 hrs.) at 260 atm., 400.degree., a space velocity of 1.2 kg./l./hr., and a H consumption of 2.5%, and yields 62.8% diesel fuel, 16.6% spindle oil, 15.3% paraffin wax, and 98.1% total liquid products. Hydrocracking of the product from hydrotreating, using an addnl. 1.8% H, gives under the same operating conditions 11.4% light gasoline, 36.9% aviation kerosine (grade TS-1), 31.7% diesel fuel (pour point -10.degree.), and total liquid

products 90.9%.

IT 7782-44-7, Oxygen
 (compds., **hydrogenation** of, in shale oil)
 RN 7782-44-7 HCA
 CN Oxygen (8CI, 9CI) (CA INDEX NAME)

O=O

CC 22 (Petroleum, Lubricants, and Asphalt)
 IT Gasoline
 (by **hydrogenation**, of shale oil)
 IT Kerosine
 (from **hydrogenated** shale oil)
 IT Hydrocarbons
 (**hydrogenation** of aromatic, and hydrocracking of heavy,
 in shale oil)
 IT Asphalt
 (**hydrogenation** of shale-oil)
 IT Shale oils
 (**hydrogenation** of, by catalysts)
 IT Olefins
 (**hydrogenation** of, in shale oil)
 IT Catalysts
 (in **hydrogenation**, of shale oil)
 IT Alkanes
 (isomerization of, in **hydrogenation** of shale oil)
 IT Isomerization
 (of paraffins, in **hydrogenation** of shale oil)
 IT **Hydrogenation**
 (of shale oils)
 IT 13762-14-6, Cobalt molybdate(VI), CoMoO4
 (catalysts from Al2O3 and, in **hydrogenation** of shale
 oil)
 IT 12138-09-9, Tungsten sulfide, WS2 16812-54-7, **Nickel**
 sulfide, NiS
 (catalysts from Al2O3, in **hydrogenation** of
 shale oil)
 IT 7440-44-0, Carbon
 (catalysts from MoS2 and, in **hydrogenation** of shale
 oil)
 IT 1317-33-5, Molybdenum sulfide, MoS2
 (catalysts, in **hydrogenation** of shale oil)
 IT 7727-37-9, Nitrogen
 (compds., **hydrogenation** in acids, in shale oil)
 IT 7704-34-9, Sulfur 7782-44-7, Oxygen
 (compds., **hydrogenation** of, in shale oil)

=> d his 173-

FILE 'HCA'

L73 1070 S (TITANIUM# OR TI) (2A) SILICALITE#
L74 51 S L73 AND L20 AND L21
L75 29 S L74 AND (L29 OR L32)
L76 12 S L75 NOT (L65 OR L66 OR L67)
L77 10 S L75 NOT (L65 OR L66 OR L67 OR L72)

=> d 177 1-10 cbib abs hitstr hitind

L77 ANSWER 1 OF 10 HCA COPYRIGHT 2006 ACS on STN

143:442977 Preparation of **hydrogen peroxide**

solutions and their use for oxidation and epoxidation reactions.

Haas, Thomas; Stochniol, Guido; Jahn, Robert (Degussa A.-G., Germany). PCT Int. Appl. WO 2005108285 A1 20051117, 23 pp.

DESIGNATED STATES: W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IS, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG, TR. (English). CODEN: PIXXD2. APPLICATION: WO 2005-EP3933 20050414. PRIORITY: DE 2004-102004023766 20040511.

AB Org. or aq.-org. **hydrogen peroxide** solns. are prepd. by direct synthesis from a nonexplosive **gaseous** mixt. contg. **hydrogen** and oxygen, in the presence of a noble metal catalyst, using a reaction medium contg. a halide and a strong acid. The reaction can be carried out in a stainless steel reactor without corrosion occurring on the reactor material if, during the reaction, the surface of the stainless steel is at no point in permanent contact with the gaseous mixt. passing through the reactor. The reaction medium is an alc., preferably methanol. The prepd. solns. are used for the catalytic oxidn. of org. substrates, such as olefins, or arom. hydrocarbons, in the presence of an oxidn. catalyst, such as **titanium silicalite**, vanadium, molybdenum, or tungsten compds. Preferably, the solns. are used for the epoxidn. of propene in the presence of **titanium silicalite** as a catalyst.

IT 7722-84-1P, **Hydrogen peroxide**, preparation

(oxidant; prepn. of **hydrogen peroxide** solns. and their use for oxidn. and epoxidn. reactions)

RN 7722-84-1 HCA
 CN Hydrogen peroxide (H2O2) (9CI) (CA INDEX NAME)

HO-OH

IT 1333-74-0, Hydrogen, reactions 7782-44-7, Oxygen,
 reactions
 (prepn. of **hydrogen peroxide** solns. and their
 use for oxidn. and epoxidn. reactions)

RN 1333-74-0 HCA
 CN Hydrogen (8CI, 9CI) (CA INDEX NAME)

H-H

RN 7782-44-7 HCA
 CN Oxygen (8CI, 9CI) (CA INDEX NAME)

O=O

IC ICM C01B015-029
 ICS B01J008-02; B01J008-00; B01J019-00
 CC 49-8 (Industrial Inorganic Chemicals)
 Section cross-reference(s): 45, 55, 67
 ST **hydrogen peroxide** prodn hydrogen oxygen bubble
 column reactor; oxidn epoxidn propene **hydrogen**
peroxide soln methanol
 IT Reactors
 (bubble column; prepn. of **hydrogen peroxide**
 solns. and their use for oxidn. and epoxidn. reactions)
 IT Oxidation
 (catalytic; prepn. of **hydrogen peroxide**
 solns. and their use for oxidn. and epoxidn. reactions)
 IT Corrosion
 (pitting; prepn. of **hydrogen peroxide** solns.
 and their use for oxidn. and epoxidn. reactions)
 IT Epoxidation
 Oxidation catalysts
 (prepn. of **hydrogen peroxide** solns. and their
 use for oxidn. and epoxidn. reactions)
 IT **Titanium silicalite**
 (prepn. of **hydrogen peroxide** solns. and their
 use for oxidn. and epoxidn. reactions)
 IT Columns and Towers
 (reactor bubble; prepn. of **hydrogen peroxide**
 solns. and their use for oxidn. and epoxidn. reactions)

- IT 11107-04-3, V4A
(V4A stainless steel, reactor material; prepn. of **hydrogen peroxide** solns. and their use for oxidn. and epoxidn. reactions)
- IT 1344-28-1, Alumina, uses
(catalyst support; prepn. of **hydrogen peroxide** solns. and their use for oxidn. and epoxidn. reactions)
- IT 115-07-1, Propene, reactions
(epoxidn.; prepn. of **hydrogen peroxide** solns. and their use for oxidn. and epoxidn. reactions)
- IT 7722-84-1P, **Hydrogen peroxide**, preparation
(oxidant; prepn. of **hydrogen peroxide** solns. and their use for oxidn. and epoxidn. reactions)
- IT 7439-98-7D, Molybdenum, compds. 7440-05-3, Palladium, uses 7440-33-7D, Tungsten, compds. 7440-57-5, Gold, uses 7440-62-2D, Vanadium, compds.
(prepn. of **hydrogen peroxide** solns. and their use for oxidn. and epoxidn. reactions)
- IT 75-56-9P, Propylene oxide, preparation
(prepn. of **hydrogen peroxide** solns. and their use for oxidn. and epoxidn. reactions)
- IT 7647-15-6, Sodium bromide, **processes** 7664-93-9, Sulfuric acid, **processes**
(prepn. of **hydrogen peroxide** solns. and their use for oxidn. and epoxidn. reactions)
- IT 1333-74-0, Hydrogen, reactions 7782-44-7, Oxygen, reactions
(prepn. of **hydrogen peroxide** solns. and their use for oxidn. and epoxidn. reactions)
- IT 67-56-1, Methanol, uses
(solvent; prepn. of **hydrogen peroxide** solns. and their use for oxidn. and epoxidn. reactions)
- L77 ANSWER 2 OF 10 HCA COPYRIGHT 2006 ACS on STN
143:288871 **Process** for making **hydrogen peroxide**. Le-Khac, Bi; Grey, Roger A. (USA). U.S. Pat. Appl. Publ. US 2005201925 A1 20050915, 7 pp. (English). CODEN: USXXCO. APPLICATION: US 2004-796810 20040309.
- AB A **process** for making **hydrogen peroxide** directly from hydrogen and oxygen is disclosed. The process comprises reacting the gases in a solvent in the presence of a catalyst comprising a polymer-encapsulated transition metal. Polymer-encapsulated transition metal catalysts are easy to prep. and use, they are easy to recover and reuse, and they provide good conversions to **hydrogen peroxide**.
- IT 1333-74-0, **Hydrogen**, reactions 7782-44-7, **Oxygen**, reactions

(**process** for making **hydrogen peroxide**
)

RN 1333-74-0 HCA

CN Hydrogen (8CI, 9CI) (CA INDEX NAME)

H-H

RN 7782-44-7 HCA

CN Oxygen (8CI, 9CI) (CA INDEX NAME)

O=O

IT 7722-84-1P, **Hydrogen peroxide**,
preparation

(**process** for making **hydrogen peroxide**
)

RN 7722-84-1 HCA

CN Hydrogen peroxide (H2O2) (9CI) (CA INDEX NAME)

HO-OH

IC ICM C01B015-029

INCL 423584000

CC 49-8 (Industrial Inorganic Chemicals)

ST **hydrogen peroxide** manuf

IT Alcohols, processes

(C1-4; **process** for making **hydrogen peroxide**)

IT Catalysts

(contg. polymer-encapsulated metal; **process** for making
hydrogen peroxide)

IT Acrylic polymers, uses

Fluoropolymers, uses

Peptides, uses

Polyamides, uses

Polyesters, uses

Polynucleotides

Polyolefins

Polysaccharides, uses

Polyureas

Polyurethanes, uses

(encapsulation material for metal catalyst; **process** for
making **hydrogen peroxide**)

IT Catalyst supports

Solvents

- (process for making hydrogen peroxide
)
- IT Aluminates
Clays, uses
Silicates, uses
Titanium silicalite
Transition metals, uses
Zeolites (synthetic), uses
(process for making hydrogen peroxide
)
- IT Acids, processes
(process for making hydrogen peroxide
)
- IT 9003-53-6, Polystyrene
(encapsulation material for metal catalyst; process for
making hydrogen peroxide)
- IT 7439-89-6, Iron, uses 7440-02-0, Nickel, uses 7440-05-3,
Palladium, uses 7440-06-4, Platinum, uses 7440-15-5, Rhenium,
uses 7440-16-6, Rhodium, uses 7440-18-8, Ruthenium, uses
7440-44-0, Carbon, uses 7440-48-4, Cobalt, uses 7440-57-5, Gold,
uses
(process for making hydrogen peroxide
)
- IT 67-56-1, Methanol, processes 124-38-9, Carbon dioxide, processes
7664-38-2, Phosphoric acid, processes 10035-10-6, Hydrogen
bromide, processes
(process for making hydrogen peroxide
)
- IT 1333-74-0, Hydrogen, reactions 7782-44-7
, Oxygen, reactions
(process for making hydrogen peroxide
)
- IT 7722-84-1P, Hydrogen peroxide,
preparation
(process for making hydrogen peroxide
)
- L77 ANSWER 3 OF 10 HCA COPYRIGHT 2006 ACS on STN
- 142:137759 Intermediate precursor compositions used to make supported
reactive catalysts having a controlled coordination structure and
methods for preparing such compositions. Zhou, Bing; Rueter,
Michael A. (USA). U.S. Pat. Appl. Publ. US 2005014636 A1 20050120,
25 pp. (English). CODEN: USXXCO. APPLICATION: US 2003-618909
20030714.
- AB The precursor compns. include a catalyst complex formed from
catalyst atoms and a control agent (which contains a polymer, e.g.,
polyacrylic acid) that is applied to a substrate. Redn. of the
catalyst complex yields supported reactive catalyst in which a

preponderance of the top or outer layer of atoms of the catalyst particles exhibit a controlled coordination no. of 2. The supported catalysts are useful for a variety of chem. reactions, including the prepn. of **hydrogen peroxide** with high selectivity.

IT **7722-84-1P, Hydrogen peroxide,**
preparation

(method for prepg. intermediate precursor compns. used to make supported reactive catalysts having controlled coordination structure)

RN 7722-84-1 HCA

CN Hydrogen peroxide (H2O2) (9CI) (CA INDEX NAME)

HO-OH

IT **1333-74-0, Hydrogen, reactions 7782-44-7, Oxygen,**
reactions

(method for prepg. intermediate precursor compns. used to make supported reactive catalysts having controlled coordination structure)

RN 1333-74-0 HCA

CN Hydrogen (8CI, 9CI) (CA INDEX NAME)

H-H

RN 7782-44-7 HCA

CN Oxygen (8CI, 9CI) (CA INDEX NAME)

O=O

IC ICM C08F020-02

ICS B01J031-00

INCL 502159000; 525329700; 502150000; 502155000

CC 49-8 (Industrial Inorganic Chemicals)

Section cross-reference(s): 37, 67

ST supported reactive catalyst intermediate precursor compn control agent; polyacrylic acid contg control agent supported reactive catalyst; **hydrogen peroxide** manuf supported reactive catalyst

IT **Titanium silicalite**

(support; method for prepg. intermediate precursor compns. used to make supported reactive catalysts having controlled coordination structure)

IT **7722-84-1P, Hydrogen peroxide,**
preparation

(method for prepg. intermediate precursor compns. used to make supported reactive catalysts having controlled coordination structure)

IT 1333-74-0, Hydrogen, reactions 7782-44-7, Oxygen, reactions

(method for prepg. intermediate precursor compns. used to make supported reactive catalysts having controlled coordination structure)

L77 ANSWER 4 OF 10 HCA COPYRIGHT 2006 ACS on STN

139:261634 Process for the epoxidation of olefins with **hydrogen peroxide** in the manufacture of epoxides. Hofen, Willi; Thiele, Georg; Haas, Thomas; Woell, Wolfgang; Kampeis, Percy; Kolbe, Baerbel (Degussa A.-G., Germany; Uhde G.m.b.H.). Eur. Pat. Appl. EP 1346986 A1 20030924, 10 pp. DESIGNATED STATES: R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR. (English). CODEN: EPXXDW. APPLICATION: EP 2002-6080 20020318.

AB A process for the catalytic epoxidn. of olefins in at least one reaction stage comprises: (a) reacting the olefin (e.g., propylene) with **hydrogen peroxide** in an org., water-miscible solvent (e.g., methanol) in the presence of a **titanium silicalite** catalyst (e.g., an MFI zeolite) in a reactor while continuously feeding an inert gas stream into the reactor; (b) continuously removing an exit gas stream contg. olefin oxide (e.g., propylene oxide), unreacted olefin, **oxygen** and inert **gas** from the reactor; (c) bringing the exit gas stream into contact in an absorption unit with the same solvent as used in the reaction stage; (d) removing a solvent stream loaded with olefin and olefin oxide from the absorption unit; and (e) discharging a **gas stream** contg. **oxygen** and the inert gas from the absorption unit. A process flow diagram is presented.

IT 7782-44-7P, Oxygen, preparation
(in a process for the epoxidn. of olefins with **hydrogen peroxide** in the manuf. of epoxides)

RN 7782-44-7 HCA

CN Oxygen (8CI, 9CI) (CA INDEX NAME)

O=O

IT 7722-84-1, **Hydrogen peroxide**, reactions
(**process** for the epoxidn. of olefins with **hydrogen peroxide** in the manuf. of epoxides)

RN 7722-84-1 HCA

CN Hydrogen peroxide (H2O2) (9CI) (CA INDEX NAME)

HO-OH

- IC ICM C07D301-12
ICS C07D301-32
- CC 35-2 (Chemistry of Synthetic High Polymers)
Section cross-reference(s): 27, 48
- ST alkene **hydrogen peroxide** epoxidn manuf epoxide
titanium silicalite catalyst; propylene
hydrogen peroxide epoxidn methyloxirane manuf
titanium silicalite catalyst; propene
hydrogen peroxide epoxidn methyloxirane manuf
titanium silicalite catalyst
- IT Columns and Towers
(absorption columns; in a process for the epoxidn. of olefins
with **hydrogen peroxide** in the manuf. of
epoxides)
- IT Columns and Towers
(bubble; in a process for the epoxidn. of olefins with
hydrogen peroxide in the manuf. of epoxides)
- IT Absorption apparatus
(column; in a process for the epoxidn. of olefins with
hydrogen peroxide in the manuf. of epoxides)
- IT Ethers, uses
(cyclic, solvents; in a process for the epoxidn. of olefins with
hydrogen peroxide in the manuf. of epoxides)
- IT **Titanium silicalite**
(epoxidn. catalyst; in a process for the epoxidn. of olefins with
hydrogen peroxide in the manuf. of epoxides)
- IT Zeolite ZSM-11
Zeolite ZSM-5
(epoxidn. catalysts in a process for the epoxidn. of olefins with
hydrogen peroxide in the manuf. of epoxides)
- IT Glycols, uses
(ethers, solvents; in a process for the epoxidn. of olefins with
hydrogen peroxide in the manuf. of epoxides)
- IT Ethers, uses
(glycol, solvents; in a process for the epoxidn. of olefins with
hydrogen peroxide in the manuf. of epoxides)
- IT Epoxidation
(process for the epoxidn. of olefins with **hydrogen**
peroxide in the manuf. of epoxides)
- IT Epoxides
(process for the epoxidn. of olefins with **hydrogen**
peroxide in the manuf. of epoxides)
- IT Alkenes, reactions
(process for the epoxidn. of olefins with **hydrogen**
peroxide in the manuf. of epoxides)

- IT Nozzles
(ring nozzles; in a process for the epoxidn. of olefins with **hydrogen peroxide** in the manuf. of epoxides)
- IT Alcohols, uses
Glycols, uses
Ketones, uses
(solvents; in a process for the epoxidn. of olefins with **hydrogen peroxide** in the manuf. of epoxides)
- IT Epoxidation catalysts
(**titanium silicalite** in a process for the epoxidn. of olefins with **hydrogen peroxide** in the manuf. of epoxides)
- IT Reactors
(trickle-bed; in a process for the epoxidn. of olefins with **hydrogen peroxide** in the manuf. of epoxides)
- IT 7782-44-7P, Oxygen, preparation
(in a process for the epoxidn. of olefins with **hydrogen peroxide** in the manuf. of epoxides)
- IT 115-07-1, Propene, reactions
(in a process for the epoxidn. of olefins with **hydrogen peroxide** in the manuf. of epoxides)
- IT 75-56-9P, Methyloxirane, preparation
(process for the epoxidn. of olefins with **hydrogen peroxide** in the manuf. of epoxides)
- IT 7722-84-1, **Hydrogen peroxide**, reactions
(process for the epoxidn. of olefins with **hydrogen peroxide** in the manuf. of epoxides)
- IT 67-56-1, Methanol, uses
(solvent; in a process for the epoxidn. of olefins with **hydrogen peroxide** in the manuf. of epoxides)
- L77 ANSWER 5 OF 10 HCA COPYRIGHT 2006 ACS on STN
138:340423 Direct synthesis of **hydrogen peroxide** and integration of the process into oxidation processes. Haas, Thomas; Stochniol, Guido; Rollmann, Jurgen (Degussa AG, Germany). U.S. Pat. Appl. Publ. US 2003083510 A1 20030501, 6 pp. (English). CODEN: USXXCO. APPLICATION: US 2002-254746 20020925. PRIORITY: DE 2001-10153546 20011030.
- AB Aq.-org. or org. **hydrogen peroxide** solns. can be produced by direct synthesis in the presence of a catalyst fixed bed and an org. solvent. According to the invention, a non-explosive gas mixt. comprising **H2** and **O2** is employed and a liq. reaction medium comprising org. solvent and bromide and/or iodide is passed over the fixed bed with a cross-section loading of at least 0.3 m/h. In the case of a trickle bed procedure with a cross-section loading of 0.3 m/h to 2 m/h, 4 to 10 wt.% methanolic **H2O2** solns. can be prepd. with a high productivity.
- IT 1333-74-0, **Hydrogen**, processes

7782-44-7, Oxygen, processes

(direct synthesis of **hydrogen peroxide** and
integration of process into oxidn. processes)

RN 1333-74-0 HCA

CN Hydrogen (8CI, 9CI) (CA INDEX NAME)

H-H

RN 7782-44-7 HCA

CN Oxygen (8CI, 9CI) (CA INDEX NAME)

O=O

IT **7722-84-1P, Hydrogen peroxide,**
preparation

(direct synthesis of **hydrogen peroxide** and
integration of process into oxidn. processes)

RN 7722-84-1 HCA

CN Hydrogen peroxide (H2O2) (9CI) (CA INDEX NAME)

HO-OH

IC ICM C01B015-01

ICS C07D301-12

INCL 549531000; 423584000

CC 49-8 (Industrial Inorganic Chemicals)

ST **hydrogen peroxide** direct synthesis integration
oxidn process

IT Oxidation

Oxidation catalysts

(direct synthesis of **hydrogen peroxide** and
integration of process into oxidn. processes)

IT Noble metals

Silicalites (zeolites)

Titanium silicalite

Zeolites (synthetic), uses

(direct synthesis of **hydrogen peroxide** and
integration of process into oxidn. processes)

IT Alkenes, processes

Aromatic hydrocarbons, processes

Sulfonic acids, processes

(direct synthesis of **hydrogen peroxide** and
integration of process into oxidn. processes)

IT Alcohols, uses

(direct synthesis of **hydrogen peroxide** and

- integration of process into oxidn. processes)
- IT 1314-23-4, Zirconia, uses 1344-28-1, Alumina, uses 7439-88-5, Iridium, uses 7440-05-3, Palladium, uses 7440-16-6, Rhodium, uses 7440-18-8, Ruthenium, uses 7440-22-4, Silver, uses 7440-50-8, Copper, uses 7440-57-5, Gold, uses 7440-62-2, Vanadium, uses 7631-86-9, Silica, uses 13463-67-7, Titania, uses (direct synthesis of **hydrogen peroxide** and integration of process into oxidn. processes)
- IT 1333-74-0, **Hydrogen, processes** 7647-01-0, Hydrochloric acid, processes 7782-44-7, **Oxygen, processes** 13598-36-2, Phosphonic acid 24959-67-9, Bromide, processes (direct synthesis of **hydrogen peroxide** and integration of process into oxidn. processes)
- IT 7722-84-1P, **Hydrogen peroxide**, preparation (direct synthesis of **hydrogen peroxide** and integration of process into oxidn. processes)
- IT 64-17-5, Ethanol, uses 67-56-1, Methanol, uses 71-23-8, n-Propanol, uses 71-36-3, n-Butanol, uses 7647-15-6, Sodium bromide, uses 7664-93-9, Sulfuric acid, uses (direct synthesis of **hydrogen peroxide** and integration of process into oxidn. processes)

L77 ANSWER 6 OF 10 HCA COPYRIGHT 2006 ACS on STN

138:172784 Synthesis of **hydrogen peroxide** from oxygen and hydrogen using a catalyst. Paparatto, Giuseppe; De Alberti, Giordano; D'Aloisio, Rino; Buzzoni, Roberto (ENI S.p.A., Italy; Polimeri Europa S.p.A.). PCT Int. Appl. WO 2003014014 A2 20030220, 31 pp. DESIGNATED STATES: W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG, TR. (English). CODEN: PIXXD2. APPLICATION: WO 2002-EP8546 20020730. PRIORITY: IT 2001-MI1688 20010802.

AB A catalyst useful for the synthesis of **hydrogen peroxide** starting from hydrogen and oxygen consists of at least one metal of the platinum group as active component, a polyolefin, and a carrier. The catalyst contains 0.05-2 wt.% of Pd, 0.005-0.5 wt.% of Pt with an at. ratio of Pt/Pd of (1-30)/(70-99), and optionally Ru, Rh, Ir, and Au. The polyolefins can be rubbers and copolymers of butadiene-styrene (synthetic rubber; GRS, SBR); ethylenepropylene (EPM, EPR) copolymers, ethylenepropylenediene copolymers (EPDM rubbers), styrene-butadiene-styrene (SBR

thermoplastic rubbers); isobutylene isoprene rubber (butylrubbers). The carrier can be silica, alumina, silica-alumina, zeolites, and preferably activated carbon or activated carbon functionalized with sulfonic groups with a surface area of > 600 m²/g. The catalyst is prepd. by dispersing the precursors of the single metal components on an inert carrier which can be pretreated with a polyolefin by pptn. or impregnation. The reaction solvent contains a halogenated promoter, such as HBr, NaBr, KBr, or NH₄Br, and/or an acid promoter, such as sulfuric, phosphoric, nitric acid or sulfonic acids. The solvent consists of at least one alc. or a mixt. of alc.-water optionally contg. an aliph. ether and/or one or more C₅-32 hydrocarbons. The alc. can be ethanol, tert. butanol, or preferably methanol. The ether is Me tert-Bu ether. The hydrocarbon is selected from paraffins, such as n-hexane, n-heptane, n-octane, and n-decane, cyclo-paraffinic hydrocarbons, such as cyclohexane, decalin, methylcyclohexane, ethylcyclohexane and dimethylcyclohexane, arom. hydrocarbons, such as benzene, naphthalene, toluene, xylenes, ethylbenzene, cumene, and alkyl naphthalenes. The reaction is carried out at 20-40.degree.C, 30-100 bars, and in the presence of an inert gas, such as N₂, He, or Ar. The produced **hydrogen peroxide** soln. can be directly used in an oxidn. process of a substrate, e.g. olefins, arom. hydrocarbons, ammonia, and carbonyl compds., catalyzed by **titanium silicalite**.

IT 7722-84-1P, **Hydrogen peroxide**,
preparation
(synthesis of **hydrogen peroxide** from oxygen
and hydrogen using catalyst)
RN 7722-84-1 HCA
CN Hydrogen peroxide (H₂O₂) (9CI) (CA INDEX NAME)

HO-OH

IT 1333-74-0, Hydrogen, reactions 7782-44-7, Oxygen,
reactions
(synthesis of **hydrogen peroxide** from oxygen
and hydrogen using catalyst)
RN 1333-74-0 HCA
CN Hydrogen (8CI, 9CI) (CA INDEX NAME)

H-H

RN 7782-44-7 HCA
CN Oxygen (8CI, 9CI) (CA INDEX NAME)

O=O

IC ICM C01B015-00
CC 49-3 (Industrial Inorganic Chemicals)
Section cross-reference(s): 45, 67
ST **hydrogen peroxide** prodn oxygen oxidn catalyst
polyolefin transition metal; hydrocarbon oxidn **hydrogen**
peroxide titanium silicalite catalyst
IT Sulfonic acids, uses
(acid promoter; synthesis of **hydrogen peroxide**
from oxygen and hydrogen using catalyst)
IT Isoprene-styrene rubber
(block; synthesis of **hydrogen peroxide** from
oxygen and hydrogen using catalyst)
IT Zeolites (synthetic), uses
(catalyst support; synthesis of **hydrogen**
peroxide from oxygen and hydrogen using catalyst)
IT Isoprene-styrene rubber
(**hydrogenated**, block; synthesis of **hydrogen**
peroxide from oxygen and hydrogen using catalyst)
IT Alkenes, reactions
Carbonyl compounds (organic), reactions
(oxidn. of; synthesis of **hydrogen peroxide**
from oxygen and hydrogen using catalyst)
IT Aromatic hydrocarbons, reactions
(solvent, oxidn. of; synthesis of **hydrogen**
peroxide from oxygen and hydrogen using catalyst)
IT Alkanes, uses
(solvent; synthesis of **hydrogen peroxide** from
oxygen and hydrogen using catalyst)
IT Alcohols, uses
(solvent; synthesis of **hydrogen peroxide** from
oxygen and hydrogen using catalyst)
IT Oxidation catalysts
(synthesis of **hydrogen peroxide** from oxygen
and hydrogen using catalyst)
IT Butyl rubber, uses
EPDM rubber
Ethylene-propylene rubber
Isoprene rubber, uses
Polyolefin rubber
Polyolefins
Styrene-butadiene rubber, uses
Titanium silicalite
(synthesis of **hydrogen peroxide** from oxygen
and hydrogen using catalyst)

- IT 7664-38-2, Phosphoric acid, uses 7664-93-9, Sulfuric acid, uses
7697-37-2, Nitric acid, uses
(acid promoter; synthesis of **hydrogen peroxide**
from oxygen and hydrogen using catalyst)
- IT 9010-85-9
(butyl rubber, synthesis of **hydrogen peroxide**
from oxygen and hydrogen using catalyst)
- IT 1344-28-1, Alumina, uses 7440-44-0, Carbon, uses 7440-44-0D,
Carbon, functionalized with sulfonic groups 7631-86-9, Silica,
uses 159995-97-8, Aluminum silicon oxide
(catalyst support; synthesis of **hydrogen**
peroxide from oxygen and hydrogen using catalyst)
- IT 9010-79-1
(ethylene-propylene rubber, synthesis of **hydrogen**
peroxide from oxygen and hydrogen using catalyst)
- IT 7647-15-6, Sodium bromide (NaBr), uses 7758-02-3, Potassium
bromide (KBr), uses 10035-10-6, Hydrogen bromide, uses
12124-97-9, Ammonium bromide (NH₄Br)
(halogenated promoter; synthesis of **hydrogen**
peroxide from oxygen and hydrogen using catalyst)
- IT 9003-31-0
(isoprene rubber, synthesis of **hydrogen**
peroxide from oxygen and hydrogen using catalyst)
- IT 105729-79-1
(isoprene-styrene rubber, block; synthesis of **hydrogen**
peroxide from oxygen and hydrogen using catalyst)
- IT 7664-41-7, Ammonia, reactions
(oxidn. of; synthesis of **hydrogen peroxide**
from oxygen and hydrogen using catalyst)
- IT 71-43-2, Benzene, uses 91-17-8, Decaline 91-20-3, Naphthalene,
uses 91-20-3D, Naphthalene, alkyl derivs. 98-82-8, Cumene
100-41-4, Ethylbenzene, uses 108-87-2, Methylcyclohexane
108-88-3, Toluene, uses 110-54-3, n-Hexane, uses 110-82-7,
Cyclohexane, uses 111-65-9, n-Octane, uses 124-18-5, n-Decane
142-82-5, n-Heptane, uses 1330-20-7, Xylene, uses 1634-04-4,
Methyl tert-butyl ether 1678-91-7, Ethylcyclohexane 27195-67-1,
Dimethylcyclohexane
(solvent; synthesis of **hydrogen peroxide** from
oxygen and hydrogen using catalyst)
- IT 64-17-5, Ethanol, uses 67-56-1, Methanol, uses 75-65-0, tert.
Butanol, uses 7732-18-5, Water, uses
(solvent; synthesis of **hydrogen peroxide** from
oxygen and hydrogen using catalyst)
- IT 9003-55-8
(styrene-butadiene rubber, synthesis of **hydrogen**
peroxide from oxygen and hydrogen using catalyst)
- IT 7439-88-5, Iridium, uses 7440-05-3, Palladium, uses 7440-06-4,
Platinum, uses 7440-16-6, Rhodium, uses 7440-18-8, Ruthenium,

uses 7440-57-5, Gold, uses 9002-88-4, Polyethylene 9003-07-0, Polypropylene 9003-17-2, Polybutadiene 9003-53-6, Polystyrene 9003-55-8, Butadiene-styrene copolymer 9010-79-1, Ethylene propylene copolymer

(synthesis of **hydrogen peroxide** from oxygen and hydrogen using catalyst)

IT 7722-84-1P, **Hydrogen peroxide**, preparation

(synthesis of **hydrogen peroxide** from oxygen and hydrogen using catalyst)

IT 7440-37-1, Argon, uses 7440-59-7, Helium, uses 7727-37-9, Nitrogen, uses

(synthesis of **hydrogen peroxide** from oxygen and hydrogen using catalyst)

IT 1333-74-0, Hydrogen, reactions 7782-44-7, Oxygen, reactions

(synthesis of **hydrogen peroxide** from oxygen and hydrogen using catalyst)

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133:43954 Integrated process for the manufacture of epoxides from olefins. Vogtel, Peter; Dorf, Ernst-Ulrich; Wegener, Gerhard; Weisbeck, Markus (Bayer A.-G., Germany). Ger. Offen. DE 19857137 A1 20000615, 7 pp. (German). CODEN: GWXXBX. APPLICATION: DE 1998-19857137 19981211.

AB Dil. **H2O2** solns. are prepd. from elemental H and O in a first step using a Pd catalyst and converted in a subsequent liq.-phase epoxidn. with olefin (esp. propylene) in the presence of **Ti silicalite** to epoxidized olefins, and the solvents are recycled into the **H2O2** formation process.

IT 7722-84-1P, **Hydrogen peroxide**, preparation

(integrated **process** for **hydrogen peroxide** prepn. in dil. soln. and use in epoxidn. of olefins)

RN 7722-84-1 HCA

CN Hydrogen peroxide (H2O2) (9CI) (CA INDEX NAME)

HO-OH

IT 1333-74-0, Hydrogen, reactions 7782-44-7, Oxygen, reactions

(integrated **process** for **hydrogen peroxide** prepn. in dil. soln. and use in epoxidn. of olefins)

RN 1333-74-0 HCA

CN Hydrogen (8CI, 9CI) (CA INDEX NAME)

H-H

RN 7782-44-7 HCA
CN Oxygen (8CI, 9CI) (CA INDEX NAME)

O=O

IC ICM C07D301-10
CC 35-2 (Chemistry of Synthetic High Polymers)
Section cross-reference(s): 27, 45
IT Epoxidation
(integrated **process** for **hydrogen peroxide** prepn. in dil. soln. and use in epoxidn. of olefins)
IT **Titanium silicalite**
(integrated **process** for **hydrogen peroxide** prepn. in dil. soln. and use in epoxidn. of olefins)
IT Alkenes, reactions
(integrated **process** for **hydrogen peroxide** soln. prepn. and use in epoxidn. of olefins)
IT 7440-05-3, Palladium, uses
(integrated **process** for **hydrogen peroxide** prepn. in dil. soln. and use in epoxidn. of olefins)
IT 7722-84-1P, **Hydrogen peroxide**, preparation
(integrated **process** for **hydrogen peroxide** prepn. in dil. soln. and use in epoxidn. of olefins)
IT 1333-74-0, **Hydrogen**, reactions 7782-44-7
, **Oxygen**, reactions
(integrated **process** for **hydrogen peroxide** prepn. in dil. soln. and use in epoxidn. of olefins)
IT 75-56-9P, Propylene oxide, preparation
(integrated **process** for **hydrogen peroxide** soln. prepn. and use in epoxidn. of olefins)
IT 115-07-1, Propylene, reactions
(integrated **process** for **hydrogen peroxide** soln. prepn. and use in epoxidn. of olefins)

L77 ANSWER 8 OF 10 HCA COPYRIGHT 2006 ACS on STN
132:142643 New catalyst, process for the production of **hydrogen peroxide** and its use in oxidation processes. Paparatto,

Giuseppe; D'Aloisio, Rino; De Alberti, Giordano; Furlan, Piero; Arca, Vittorio; Buzzoni, Roberto; Meda, Laura (Enichem S.p.A., Italy; Polimeri Europa S.p.A.). Eur. Pat. Appl. EP 978316 A1 20000209, 15 pp. DESIGNATED STATES: R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO. (English). CODEN: EPXXDW. APPLICATION: EP 1999-202489 19990729. PRIORITY: IT 1998-MI1843 19980805.

AB The present invention relates to a catalyst consisting of a metal of the VIII group supported on acid activated carbon functionalized with sulfonic groups, a process for the synthesis of **hydrogen peroxide** from hydrogen and oxygen which uses said catalyst and the use of the **hydrogen peroxide** soln. in oxidn. processes catalyzed by **titanium-silicalite**.

IT 7722-84-1P, **Hydrogen peroxide**, preparation

(catalyst, process for prodn. of **hydrogen peroxide** and its use in oxidn. processes)

RN 7722-84-1 HCA

CN Hydrogen peroxide (H2O2) (9CI) (CA INDEX NAME)

HO-OH

IT 1333-74-0, **Hydrogen**, reactions 7782-44-7, **Oxygen**, reactions

(catalyst, **process** for prodn. of **hydrogen peroxide** and its use in oxidn. processes)

RN 1333-74-0 HCA

CN Hydrogen (8CI, 9CI) (CA INDEX NAME)

H-H

RN 7782-44-7 HCA

CN Oxygen (8CI, 9CI) (CA INDEX NAME)

O=O

IC ICM B01J031-02

ICS B01J021-18; C01B015-029

CC 67-1 (Catalysis, Reaction Kinetics, and Inorganic Reaction Mechanisms)

Section cross-reference(s): 25, 45, 49

ST catalyst prodn **hydrogen peroxide** oxidn **process**; Group VIII metal activated carbon functionalized sulfonic group catalyst; **titanium silicalite**

- catalyst oxidn **hydrogen peroxide**
- IT Oximation catalysts
(ammoximation; catalyst, process for prodn. of **hydrogen peroxide** and its use in oxidn. processes)
- IT Epoxidation catalysts
Oxidation catalysts
(catalyst, process for prodn. of **hydrogen peroxide** and its use in oxidn. processes)
- IT Group VIII elements
Halogens
Titanium silicalite
(catalyst, process for prodn. of **hydrogen peroxide** and its use in oxidn. processes)
- IT Alkenes, reactions
(catalyst, process for prodn. of **hydrogen peroxide** and its use in oxidn. processes)
- IT Aromatic hydrocarbons, reactions
(catalyst, process for prodn. of **hydrogen peroxide** and its use in oxidn. processes)
- IT Carbonyl compounds (organic), reactions
(catalyst, process for prodn. of **hydrogen peroxide** and its use in oxidn. processes)
- IT 7429-90-5, Aluminum, uses 7439-88-5, Iridium, uses 7439-89-6, Iron, uses 7440-05-3, Palladium, uses 7440-06-4, Platinum, uses 7440-16-6, Rhodium, uses 7440-18-8, Ruthenium, uses 7440-42-8, Boron, uses 7440-44-0, Carbon, uses 7440-55-3, Gallium, uses 7447-40-7, Potassium chloride, uses 7647-14-5, Sodium chloride, uses 7647-15-6, Sodium bromide, uses 7758-02-3, Potassium bromide, uses 7789-38-0, Sodium bromate 10035-10-6, Hydrobromic acid, uses 12124-97-9, Ammonium bromide 12125-02-9, Ammonium chloride, uses
(catalyst, process for prodn. of **hydrogen peroxide** and its use in oxidn. processes)
- IT 75-56-9P, Propylene oxide, preparation **7722-84-1P**,
Hydrogen peroxide, preparation
(catalyst, process for prodn. of **hydrogen peroxide** and its use in oxidn. processes)
- IT 7446-11-9, Sulfur trioxide, processes 7664-93-9, Sulfuric acid, processes 8014-95-7, Oleum
(catalyst, process for prodn. of **hydrogen peroxide** and its use in oxidn. processes)
- IT 108-94-1, Cyclohexanone, reactions 115-07-1, Propene, reactions **1333-74-0**, **Hydrogen**, reactions 7664-41-7, Ammonia, reactions **7782-44-7**, **Oxygen**, reactions
(catalyst, **process** for prodn. of **hydrogen peroxide** and its use in oxidn. processes)

- 130:13254 Process for the selective oxidation of organic compounds.
D'Amore, Michael Brian (E. I. Du Pont de Nemours & Co., USA). PCT
Int. Appl. WO 9851811 A1 19981119, 16 pp. DESIGNATED STATES: W:
JP, US; RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU,
MC, NL, PT, SE. (English). CODEN: PIXXD2. APPLICATION: WO
1998-US8882 19980512. PRIORITY: US 1997-46709 19970516.
- AB A process for the manuf. of **oxygenated** org. compds. by
employing an oxidase to generate **H2O2** is disclosed. The
generated **H2O2** is used to oxidize an oxidizable org.
substrate in the presence of a metal-contg. catalyst. An enzyme
system of an insol. carrier of silicon oxide and an oxide of Ag, Co,
Ce, Mn, Fe, Cu, Cr, Ti, V, Mo or W, coupled with an oxidase enzyme
capable of producing **H2O2** when reacted with a **H2**
or an electron donor in the presence of **O2**, is also
disclosed.
- IT **7722-84-1P, Hydrogen peroxide,**
biological studies
(selective oxidn. of org. compds.)
- RN 7722-84-1 HCA
- CN Hydrogen peroxide (H2O2) (9CI) (CA INDEX NAME)
- HO-OH
- IC ICM C12P003-00
ICS C12P001-00; C12P017-04; C12P007-24; C07B033-00; C07B041-00;
C07D303-04; C12N011-14
- CC 16-1 (Fermentation and Bioindustrial Chemistry)
Section cross-reference(s): 21
- ST org compd oxidn oxidase **peroxide**
- IT **Titanium silicalite**
(selective oxidn. of org. compds.)
- IT **7722-84-1P, Hydrogen peroxide,**
biological studies
(selective oxidn. of org. compds.)
- L77 ANSWER 10 OF 10 HCA COPYRIGHT 2006 ACS on STN
- 129:291411 Single-step method and catalysts for producing glycol
monoethers from olefins and alcohols. Muller, Ulrich; Grosch, Georg
Heinrich; Walch, Andreas; Rieber, Norbert (BASF Aktiengesellschaft,
Germany). PCT Int. Appl. WO 9847845 A1 19981029, 16 pp. DESIGNATED
STATES: W: AL, AU, BG, BR, BY, CA, CN, CZ, GE, HU, ID, IL, JP, KR,
KZ, LT, LV, MX, NO, NZ, PL, RO, RU, SG, SI, SK, TR, UA, US, AM, AZ,
BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, CH, CY, DE, DK, ES, FI, FR,
GB, GR, IE, IT, LU, MC, NL, PT, SE. (German). CODEN: PIXXD2.
APPLICATION: WO 1998-EP2281 19980417. PRIORITY: DE 1997-19717320
19970424.
- AB Glycol monoethers (e.g., ethoxypropanols) are prepd. in high yield

and selectivity by the reaction of olefins (e.g., propylene) with an epoxidn. reagent (e.g., **hydrogen peroxide**) in the presence of a hydroxyl group-contg. org. compds. (e.g., ethanol) in a mixt. of epoxidn. catalysts (e.g., **titanium silicalite**) and alkoxylation catalysts (e.g., Lewatit).

IT 1333-74-0, Hydrogen, reactions 7722-84-1, **Hydrogen peroxide**, reactions 7782-44-7, Oxygen, reactions (single-step method and catalysts for producing glycol monoethers from olefins and alcs.)
RN 1333-74-0 HCA
CN Hydrogen (8CI, 9CI) (CA INDEX NAME)

H-H

RN 7722-84-1 HCA
CN Hydrogen peroxide (H2O2) (9CI) (CA INDEX NAME)

HO-OH

RN 7782-44-7 HCA
CN Oxygen (8CI, 9CI) (CA INDEX NAME)

O=O

IC ICM C07C043-13
ICS C07C041-05; B01J029-00
CC 45-4 (Industrial Organic Chemicals, Leather, Fats, and Waxes)
Section cross-reference(s): 23, 48, 67
IT **Titanium silicalite**
(single-step method and catalysts for producing glycol monoethers from olefins and alcs.)
IT 115-07-1, Propene, reactions 1333-74-0, Hydrogen, reactions 7722-84-1, **Hydrogen peroxide**, reactions 7782-44-7, Oxygen, reactions (single-step method and catalysts for producing glycol monoethers from olefins and alcs.)